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ABSTRACT

Methods were developed to convert data from the Regional Air Pollution/Regional Air Monitoring Study (RAPS/RAMS) into a format compatible with the Livermore Regional Air Quality (LIRAQ) models. Changes made in the LIRAQ models include (1) improved map plotting routines, (2) updated chemical mechanism, and (3) a partial SO_2 oxidation mechanism. Several appendices are intended to serve as a user's guide to the LIRAQ models and the associated data conversion routines.

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SECTION 1

FOREWORD AND INTRODUCTION

The Livermore Regional Air Quality (LIRAQ) models were developed when, through the Research Applied to National Needs (RANN) program, the National Science Foundation supported a 2½-year interagency effort by the University of California Lawrence Livermore Laboratory (LLL), the Bay Area Air Pollution Control District (BAAPCD)*, and the NASA Ames Research Center (ARC) to develop and evaluate the LIRAQ-1S and LIRAQ-2S models. These codes are deterministic two-dimensional Eulerian grid air-quality models that compute spatial and temporal distributions of significant air pollutants from specified emissions, meteorological conditions, topography, and initial and boundary concentrations.

The 1975 versions of LIRAQ-1 and LIRAQ-2 are described in a User's Guide (MacCracken, 1975), a two-volume report (MacCracken and Sauter, 1975a,b), and two journal articles (MacCracken et al., 1978; Duewer et al., 1978). The models have been further described to the potential user community at a NSF funded workshop (Sauter, 1978), by a NSF funded review (Bass et al., 1977), and in comparison with the Urban Airshed Model (UAD) (SAI, 1977; Reid and Reynolds, 1979). Evaluation and further comparison with the UAD is being funded by the U. S. Environmental Protection Agency (EPA) and carried out by the Association of Bay Area Governments (ABAG) with participation by LLL and the developers of the UAD. LIRAQ-1 deals with chemical species that are not strongly affected by chemical reactions and uses the flux-corrected transport scheme of Boris and Book (1973). LIRAQ-2 treats chemically reactive species, but uses simple upstream differencing to treat the transport.

In 1976, LLL entered into an interagency agreement with the EPA to modify and extend the LIRAQ models to include sulfur species (SO_2 and sulfates) and to prepare data processors for the necessary input files to be developed from EPA Regional Air Monitoring Study (RAMS) data tapes so that the LIRAQ models could participate in the Regional Air Pollution Study (RAPS). The improved codes are designated LIRAQ-1S and LIRAQ-2S.

This report describes: (1) the modifications made in the models, (2) the preprocessors developed to manipulate RAMS/RAPS data files and to generate LIRAQ input files from them and other user supplied inputs, (3) some of the limitations of the models as they now exist, (4) preliminary sensitivity studies, and (5) verification and future model use.

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*Now Bay Area Air Quality Management District (BAAQMD).

The appendices (Appendices A-K) of this report are designed to serve as a partial user's guide to the models. MASCON and its associated processors are documented in much greater detail in a separate user's guide (Stullich et al., 1978), and the internal structure and philosophy of the LIRAQ models are fully documented in the 1975 LIRAQ User's Guide (MacCracken et al., 1975). This report attempts to provide enough information to make it possible to execute all of the processors involved without reference to the other user's guides. However, it does not attempt to repeat the detailed content of the other user's guides, and anyone unfamiliar with the codes who intends to use them on any region except St. Louis, Missouri, is advised to read all three user's guides.

As part of the NSF contract, the models were verified for three days in the San Francisco Bay Area; two additional days have since been studied by the BAAPCD. The model verification studies for the Bay Area have demonstrated several model sensitivities, and they provide a partial basis for the evaluation of model performance.

The present EPA-supported interagency effort has consisted of a limited program intended to facilitate the examination of LIRAQ performance as part of RAPS. This effort has included only minimal model development. The bulk of the effort was spent to develop data preprocessors and operating procedures for use by remote users of LIRAQ on the Lawrence Berkeley Laboratory (LBL) computer system.

A temporary emissions inventory was provided by the EPA late in 1978. As a result, less effort than was intended has been devoted to model verification and the analysis of poorly known but important model inputs such as the specification of upper and upwind boundary conditions, and an estimate of the reliability of the procedures used in estimating mixing depths. As yet, no final emissions inventory has been established and no model tuning has been attempted. A limited set of sensitivity studies have been carried out, but are not described in this document since no funding exists to analyze the results.

SECTION 2

NUMERICAL FORMULATION OF THE LIRAQ MODEL

The LIRAQ model has two forms: LIRAQ-1S and LIRAQ-2S. LIRAQ-1S emphasizes transport, contains no chemistry, and can be run on grids with up to 45 x 50 cells. LIRAQ-2S (with a simpler transport algorithm) treats the photochemistry of a number of reactive species on a 20 x 20 cell grid.

Except for input-output (I/O), LIRAQ-1S exists unchanged from its original development; the reader is directed to MacCracken et al. (1978) and Duewer et al. (1978), or to MacCracken and Sauter (1975a,b) and MacCracken (1975) for a complete discussion of the code's numerical formulation and method of solution.

LIRAQ-2S is also basically unchanged in that the GEAR package is still used as the basis for integration of the set of coupled transport-photochemistry equations. Details of this may also be found in the above references. The addition of SO_2 and sulfate modeling capabilities into the code has necessitated some modifications to the model, and we will discuss these here.

CHEMISTRY CHANGES

In fulfillment of the contract with the EPA, it was necessary to add SO_2 and sulfate capabilities to the model. Because of storage limitations, these two species could not simply be added to the existing mechanism. Based on our understanding of the chemistry and experience with the code, four species were taken out of the dynamic calculation and instead treated as being in instantaneous chemical equilibrium with the other species. A fifth species, RNO_2, was eliminated from the calculation altogether because it had little (<1%) effect on the results. The four species that moved from dynamic to steady-state status were N_2O_5, RCO_3, RO_2, and HO_2. Table 1 lists the species treated by LIRAQ-2S. The LIRAQ-2S reaction set was modified and augmented to treat the modified set of species needed for LIRAQ-2S. There are now 56 reactions among the 20 chemical species.

TREATMENT OF STEADY-STATE SPECIES

The only complication arising from these changes is in the treatment of the steady-state species. In the 1975 version of LIRAQ-2S, it was possible to obtain an analytic expression for each of the steady state species by setting the total chemical derivatives equal to zero and solving the resulting algebraic set for the species concentrations. With four additional steady state species, this set becomes coupled and nonlinear, making an analytic solution cumbersome and impractical. The way we have dealt with the problem is to compute the chemical derivatives for the steady-state species and their variation with respect to changes in those species.

TABLE 1. Species treated by LIRAQ-2S

Dynamic species (transport-kinetics)	Instantaneous equilibrium species (kinetics only)
HC1 (alkenes)	$O(^3P)$
HC2 (alkanes)	NO_3
HC4 (aldehydes)	HO
HNO_2	RO
HNO_3	N_2O_5
H_2O_2	RCO_3
NO	RO_2
NO_2	HO_2
O_3	
CO	
SO_2	
$SO_4^=$ (sulfate)	

From these computations, new values of the steady-state species may be calculated. Because of the nonlinearities, the process must be iterative to obtain accurate solutions.

Mathematical Formulation

Mathematically, given the dynamic species concentrations Y_i at the current time and steady-state concentrations c_j at the previous time (or some initial guess), we will in general have nonzero chemical derivatives, $\dot{c}_j$, computed for the c_j. Thus,

$$\dot{c}_j = \dot{c}_j(Y_i, c_k) \tag{2-1}$$

for all j. The array $\partial \dot{c}_j / \partial c_k$ can be computed numerically. Then solutions to the equations

$$\delta \dot{c}_j = -\dot{c}_j = \sum_k \frac{\partial \dot{c}_j}{\partial c_k} \delta c_k \tag{2-2}$$

for all j, using Newton's method, will give the change of the c's required to zero their time derivatives. This will not be an exact solution because of the nonlinearities, thus the need for iteration.

Code Structure

The flow chart of the part of LIRAQ-2S associated with the steady-state and reaction calculations is shown in Figure 1.

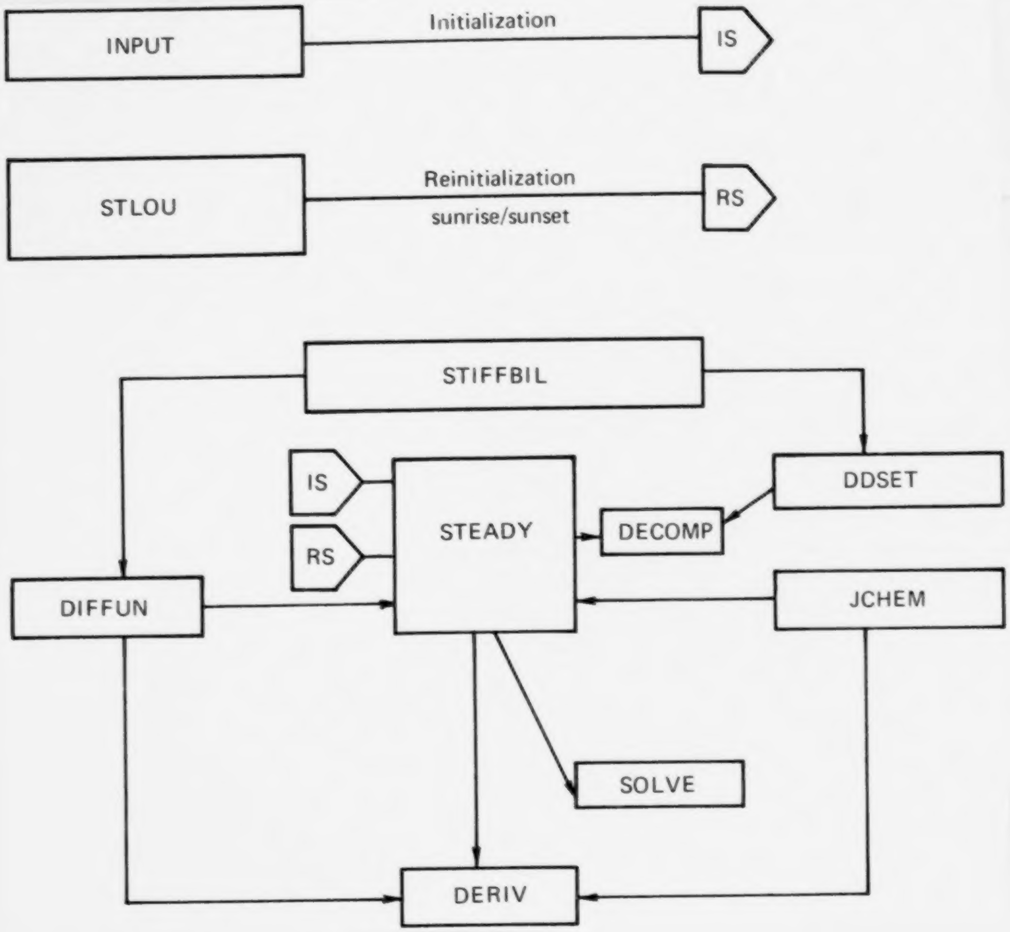
INPUT
Initialization
IS
STLOU
Reinitialization
sunrise/sunset
RS
STIFFBIL
IS
RS
STEADY
DECOMP
DDSET
DIFFUN
JCHEM
SOLVE
DERIV

FIGURE 1. LIRAQ-2 flow-chart revision.

The mathematical formulation described above is implemented in the new subroutine STEADY. In this routine, the partial derivatives $\partial \dot{c}_j/\partial c_k$ are computed and inverted using the GEAR subroutines DECOMP and SOLVE to solve Eq. (2-2) for the ∂c_k. In the integration, the $\partial \dot{c}_j/\partial c_k$ are recomputed every fifth time step to reduce computation time.

STEADY computes virtually the same set of reactions as DIFFUN and JCHEM. For this reason, and to avoid writing the same coding in three subroutines, a fourth routine (DERIV) was created that contains all the reactions. When called from DIFFUN and JCHEM, DERIV returns the chemical derivatives of the dynamic species (with the addition of the transport boundary conditions). When called from STEADY, DERIV returns the chemical derivatives of the steady-state species. In this way, changes in the LIRAQ-2S reaction mechanism need to be coded in only one place, minimizing the chance for error.

STEADY is called from DIFFUN and JCHEM as part of the integration process. STEADY is called from STIFFBIL (in the GEAR package) when it is time to update steady-state concentrations. STEADY is called from INPUT as part of the model initialization and may be called from LIRAQ-2S if reinitialization is necessitated by a sunrise or sunset.

As the integration of the equations by the GEAR package progresses, the values of the steady-state species at the previous time step are the initial guess for the iteration to new values. When a new problem is started, an initial guess must be supplied. The same is true when a sunrise or sunset occurs because these mark a discontinuous changes in the chemical derivatives and steady-state species concentrations. The subroutine INPUT includes data-loaded initial estimates (guesses) for the time of first daylight (nonzero photodissociation) and darkness (zero photodissociation). While not foolproof, the method has worked for us because of the simple form of the equations and the flexible nature of Newton's method.

A breakdown related to poorly chosen initial guesses could probably be eliminated by adjusting the values in the array YGSS(N,I) set in lines 360-370 of INPUT. The values used have led to stable solutions for a substantial range of other parameters, but this might not be the case for all possible conditions. The symptom of failure is that one or more of the steady state concentrations is calculated to be negative or infinite. See the following section for more details.

SECTION 3

INITIAL AND BOUNDARY CONDITIONS

INITIAL CONDITIONS

To start up the model, concentrations of species are needed over the entire grid. These concentrations are first introduced into LIRAQ at stations from RAPS data as is described in Appendix D. The RAPS measurements of CO, NO, NO_2, SO_2, and O_3 are accepted at face value, but the LIRAQ hydrocarbon classes in ppmV are generated from the measured ppmC concentrations of methane (CH_4) and total hydrocarbons (THC) as follows:

$$HC1 = [\text{maximum of } (THC - CH_4) \text{ or } 0.05]\ (0.2)(0.1),$$

$$HC2 = [\text{maximum of } (THC - CH_4) \text{ or } 0.05]\ (0.2)(0.87),$$

$$HC4 = [\text{maximum of } (THC - CH_4) \text{ or } 0.05]\ (0.2)(0.03).$$

The use of a minimum value of 0.05 ppmC for nonmethane hydrocarbons is designed to protect against spurious negative concentrations that might be introduced when $THC < CH_4$. The factor of 0.2 reflects an assumed mean carbon chain length of 5 for ambient nonmethane hydrocarbons early in the morning (conversion from ppmC to ppmV). The final factors are roughly those generated by the model at 0400 after a 24-hour run. They might not be suitable for initialization after about 0800 or before about 2200, because the calculated HC4 fractions typically increase in a daytime simulation, and then decline overnight.

These initial concentrations at stations are then read by the LIRAQ codes as surface concentrations. A vertical profile is deduced from the local emissions, mixing depth, wind speed, and surface concentration; from this, a mean layer concentration at the station is calculated. We then interpolate the mean layer concentrations to the grid using a Gaussian interpolation scheme and a constant of 0.1 grid squares. Any portions of the domain where the topography is above the mixing depth are then assigned the concentrations chosen for the upper-boundary condition. This method of generating initial conditions for stable species seems reasonable for the St. Louis area, but is much less reasonable for regions of complex terrain and source patterns where initialization from sparse data is a difficult problem.

The initial conditions for H_2O_2, HNO_2, HNO_3, and $SO_4^=$ are set equal to the assumed (horizontal) boundary background levels. For HNO_3 and $SO_4^=$, the choice of initial concentration does not appreciably affect any other species. For H_2O_2 and HNO_2, this is not true. QSRUN files we have used give 4.06×10^{-8} ppm (10^6 molecules/cm^3), a number that is effectively zero for these species. If the actual concentrations of HNO_2 or H_2O_2 were in the ppb range, this could significantly increase the rate of photochemical activity at sunrise. Unfortunately, there is no satisfactory way to estimate these concentrations in the absence of measurements because the attainment of the equilibrium involving HNO_2, NO, NO_2, and H_2O by homogeneous processes seems likely to take at least several hours under any conditions in the free atmosphere, and H_2O_2 should be even further from equilibrium. Alternatively, heterogeneous production or loss of HNO_2 may be rapid (especially in confined spaces with high NO_x, such as automobile exhaust pipes). We have chosen to use a low concentration for HNO_2 and H_2O_2 because there is little justification for other choices. Nevertheless, the choice of low initial concentrations for these species is itself poorly justified. The values used can readily be modified through the QSRUN file.

Initialization of the stationary-state species presents a different problem. Here, we calculate the stationary-state species from the initial dynamic species using an iterative solution for the algebraic equations. As described in Section 2, for this method to work, we start with an initial guess for the various steady-state species. Because the algebraic equations contain quadratic terms, both positive and negative solutions can exist for the steady-state species; only one solution has been found where all species are required to be positive, however. To ensure that a correct (positive) solution is reached for the steady-state species, we have found it necessary to use initial guesses for the concentrations of species appearing in quadratic terms that are significantly larger than the solutions eventually attained. Initial guesses that yield stable solutions are listed in Table 2. The most crucial estimates seem to be those for RO_2 and HO_2. An unexplained failure of a problem on initialization or at sunset might require adjustment of these initial guesses. However, they are coded into the LIRAQ-2S model and any adjustment requires recompilation of subroutine INPUTS.

BOUNDARY CONDITIONS

Boundary conditions are treated differently in LIRAQ-1S and LIRAQ-2S. In LIRAQ-1S, a concentration is read into the model for each of the four horizontal and

TABLE 2. Initial estimates for steady-state species, molecules/cm^3 (YGSS(N,I)) in subroutine INPUTS.

Species	Night (and sunset)	Day
O^3P	0.0	10^4
NO_3	10^6	10^7
HO	10^5	10^6
RO	10^6	10^6
N_2O_5	10^6	10^7
RCO_3	10^6	10^8
RO_2	10^9	10^8
HO_2	10^8	10^9

one vertical boundaries via the QSRUN file and used as the (in-flow) concentration for the boundary involved. Out-flow boundary concentrations are set to the concentration calculated at the out-flow boundary. The boundary condition for CO was set to 0.1 ppmV, a value about equal to the worldwide CO background concentration. This concentration is probably too low for use in St. Louis; estimates of background CO in the North temperate zone tend to be about 0.18 ppmV (Seiler, 1974). However, even at urban stations, RAPS measurements frequently recorded CO concentrations < 0.1 ppmV. In our opinion, this reflects an error in the RAPS measurements. The calibration techniques and instrumentation used by RAPS should have been suitable for measuring CO at the levels involved in air quality standards, but it is far from obvious that they were reliable at the sub-ppm levels actually recorded.

For SO_2, we use a background concentration of 0.01 ppmV. There is little justification for this choice except that it is roughly the lowest concentration recorded for the RAPS network for the days we examined.

LIRAQ-2S uses a more complex boundary condition:

$$C_b = (C_o^2 + \rho^2 C_i^2)^{1/2} \quad ,$$

where C_b is the inflow boundary condition, C_o is a minimum value input through QSRUN, C_i is the concentration calculated in the grid element next to the boundary, and ρ is a constant between 0 and 1 coded in for each pollutant. The values of C_o and ρ that we are currently using for the dynamic species are given in Table 3.

TABLE 3. Values of C_o and ρ for various chemical species.

Species	Horizontal boundary C_o	Upper boundary C_o	Horizontal boundaries ρ	Upper boundary ρ
O_3	0.01	0.025	0.3	0.85
HC1	0.01	0.01	0.3	0.3
HC2	0.05	0.05	0.3	0.3
HC4	0.001	0.001	0.3	0.3
HNO_2	4×10^{-8}	4×10^{-8}	0.3	0.3
HNO_3	4×10^{-8}	4×10^{-8}	0.3	0.3
H_2O_2	4×10^{-8}	4×10^{-8}	0.3	0.3
NO	0.004	0.004	0.3	0.3
NO_2	0.004	0.004	0.3	0.5
CO	0.1	0.1	0.3	0.3
SO_2	0.01	0.01	0.3	0.3
$SO_4^=$	0.001	0.001	0.3	0.3

The model is sensitive to the choices of both C_o and ρ for O_3, NO, NO_2, HC1, HC2, and HC4. Only SO_2 and $SO_4^=$, are significantly affected by the boundary conditions for SO_2 or $SO_4^=$, and the boundary conditions for HNO_3 and CO have little effect on other species. The boundary conditions used for H_2O_2 and HNO_2 reflect the absence of information and have no other justification. The values for C_o used in calculating the boundary concentrations for the other species are designed to reflect the lowest plausible concentrations reported for the area. The values of ρ are designed to permit the concentrations inside the boundary to have only a modest influence on the boundary concentrations (except for O_3 aloft where a larger influence is thought to be real). If any additional data were available (e.g., from special studies) changing C_o is very simple and is done via the input file QSRUN. Changing ρ is more difficult and involves recompiling subroutine INPUTS in LIRAQ-2S. When there is evidence for elevated O_3 concentrations aloft, we believe the choice of C_o for O_3 aloft should probably be increased (perhaps to ~ 0.08 ppm). Further, if there is any independent evidence for significant carryover of pollutants from a previous day, the C_o used for other pollutants (especially SO_2 and NO_2 aloft) might need to be increased.

In our view, the boundary concentrations of pollutants should be provided from experimental measurements on days used for model verification. The values used by us are little more than guesses made in the face of limited data. We do not view the present treatment as an integral part of the model, and if the data needed to support a more detailed prescription of the inflow boundary conditions are available, we believe they should be used.

Lest this problem be treated lightly, consider that the RAPS emissions inventory gives emissions for an area of 1.86×10^4 km^2 that, when averaged over the grid, yield 70 kg/km^2 day of NO_x, 34 kg/km^2 day of organics, 241 kg/km^2 day of CO, and 174 kg/km^2 day of SO_2. With the C_o values given in Table 3, if initialization and inflow provide a volume of 1 km^3/km^2, the C_o values would introduce 15 kg/km^2 day of NO_x, 138 kg/km^2 day of organics, 114 kg/km^2 day of CO, and 26 kg/km^2 day of SO_2. That is, boundary flow and initial conditions would dominate emissions for organics, would be comparable to emissions for CO, and would not be negligible even for SO_2 and NO_x. In the case of organic species, about 15-20% of the assumed mass from initial and boundary conditions comes through reactivity-weighted methane. The hydrocarbon composition used for initialization and boundary flow has a substantial impact on model predictions. The aldehyde concentrations used are comparable to those calculated in global models from the oxidation of methane. The alkene-like hydrocarbon concentrations are the most critical to model predictions, and the least well known. Natural sources of isoprenes and terpenes may provide a significant source of natural alkenes in many urban areas including St. Louis, although the available literature is certainly not conclusive (Sandberg et al., 1978, 1979; Zimmerman, 1977).

SECTION 4

EMISSIONS INVENTORY

The final RAPS emissions inventory has not been made avialable to us. However, an inventory said to be similar to the final inventory has been provided and used. This inventory was derived from files in the final format but has lower hydrocarbon emissions and reactivity than the current provisional inventory RAPS inventory (J. Shreffler, 1979, private communication). The processors that generated the provisional LIRAQ inventory are described in Appendix B. In this section, we discuss the special treatments that are used to generate LIRAQ compatible inventories.

HYDROCARBON SPLITTING

The available emissions inventory data contain total hydrocarbon emissions by mass and a splitting into five reactivity classes: (1) unreactive, (2) paraffin, (3) aldehyde, (4) olefin, and (5) aromatic. LIRAQ requires three hydrocarbon classes: (1) a low-reactivity class (treated as n-butane), (2) a high-reactivity class (treated as propene), and (3) a photoreactive class (treated as an aldehyde). In generating the provisional inventory, we have assumed the relations given in Table 4. These ratios are based on experience in the San Francisco Bay Area, however, and may not be completely appropriate for St. Louis.

TABLE 4. Hydrocarbon splitting factors.

HC1 = Olefin * 1.2 + Aromatic * 0.5

HC2 = Nonreactive * 0.1 + Paraffin * 1.3 + Aromatic * 0.5

HC4 = Aldehyde * 1.2

TIME CYCLE

The time variations given in the provisional RAPS inventory were used, subject to modification by a smoothing function such that the emissions rate varies sinusoidally between H-15 min and H+15 min where H is the hour covered by an hourly emissions inventory. This is done to avoid discontinuous derivatives for computed species, a numerical advantage for LIRAQ.

TREATMENT OF ELEVATED EMISSIONS

LIRAQ is a two-dimensional (horizontal) model, and as such, its treatment of elevated emissions is highly simplified. At present, LIRAQ treats all emissions from sources below 20 m as surface emissions, and all emissions from sources above 20 m as elevated emissions. Here, the determining height is stack height; plume rise is not added to the physical height although it may often be important.

Sources treated as elevated emissions are assumed to be emitted at $\sim$ 125 m. The precise treatment of these emissions is different for LIRAQ-1S and LIRAQ-2S. In LIRAQ-1S, elevated emissions are excluded if the mixing depth is $<$ 125 m. In LIRAQ-2S, elevated emissions are completely excluded if the mixing depth is $<$ 100 m and fully included if $>$ 150 m. If the mixing depth is between 100 and 150 m, LIRAQ-2S multiplies the elevated emissions by ENTRY, where $\text{ENTRY} = 0.5 \times (1 + \sin(0.02\ \pi\ (H-125))$. Here, H is the mixing depth (in meters) and all other quantities have their regular values. Again, this is done to avoid discontinuous changes in emissions.

Although it would be feasible to change the treatment of elevated emissions in LIRAQ (e.g., by introducing more than one height class of elevated source), this has not been done. This is because a two-dimensional horizontal model is not desirable for the detailed study of elevated sources (especially when considering the effect of varying stack height), and we would discourage such uses of LIRAQ. LIRAQ is primarily for predicting CO and O_3/oxidant occurrence, not for treating species like SO_2 that are emitted by elevated point sources. Although homogeneous SO_2-$SO_4^=$ chemistry has been included in a simplified way, we do not advocate the use of LIRAQ-2S as a tool for assessing SO_2 or $SO_4^=$ control strategies, especially those involving changing stack heights.

NONANTHROPOGENIC EMISSIONS AND COMPARISON OF SAN FRANCISCO BAY AREA AND INTERIM ST. LOUIS INVENTORIES

The available emissions inventories for the Bay Area and for St. Louis do not include nonanthropogenic sources. In part, nonanthropogenic emissions have been neglected because there is little data on which to base estimates of such emissions (or biogenic emissions from agriculture, etc.); in part, they have been neglected in urban areas because they have been assumed to be negligibly small in comparison with anthropogenic emissions. Unfortunately, there is little evidence to support this view, and some to contradict it.

To estimate nonanthropogenic emissions, a reasonable starting point is the review of Rasmussen et al. (1975), which provides annual average emissions of various species on global average basis. This report provides estimates of nonanthropogenic emissions of reactive hydrocarbons (based only on emissions of terpenes from forests), nonreactive hydrocarbons (based on the production of methane in swamps) (Rasmussen et al., 1975), CO (based on energy on the oxidation of methane, Seiler, 1974), NO_x (based on denitrification of soil nitrate, and N_2O oxidation), and SO_2 based on volcanic activity and oxidation of H_2S. Each of these estimates can be criticized as incomplete. There is evidence that reactive hydrocarbons are produced in wildfires, and may be produced at low levels by many plants (e.g., ethene is a known plant hormone); similar criticisms could be made about less reactive hydrocarbons. Consistent with this, nonmethane hydrocarbon concentrations of 3-10 ppb are found in the remote nonurban boundary layer (Rasmussen, 1977). NO_x is thought to be produced from lightning flashes at a rate of $\sim 10^9$ kg/y, but the estimates for NO production from N_2O, given by Rasmussen et al. (1975) appear to be based on the estimates of Bates and Hayes (1967), who used an erroneous cross section for N_2O photolysis (Johnston and Selwyn, 1975). A reasonable estimate of global NO_x production from soils, oceans, wildfires, lightning, oxidation of ammonia, etc. in the troposphere might be in the range 10^9-10^{11} kg/y. In keeping with this substantially reduced estimate of NO_x emissions, recent measurements of background NO_x concentrations over oceans and in the arctic are of the order 10^{-4}-10^{-5} ppm (Noxon, 1975; McFarland et al., 1979). Soil bacteria may be either a significant source or sink for CO. Methane oxidation and CO production from methane are unbalanced in Rasmussen's study. The CO budget estimates made by Seiler (1974) seem more reasonable than those of Rasmussen et al. (1975). The oxidation of H_2S is likely to be the major nonanthropogenic source of SO_2. When these factors are considered, the estimates given in Table 5 for nonanthropogenic emissions are deduced.

If one considers the St. Louis inventory for SO_x, NO_x, hydrocarbons, carbon monoxide, and particulate matter, one finds the values given in Table 6.

In generating the natural emissions deduced from the Rasmussen study for an area of 20,000 km^2, hydrocarbons are assumed to have sources distributed uniformly over global land areas, and we assume that CO sources are distributed uniformly over the earth, NO_x sources are assumed to be distributed uniformly either over the earth or over land, and SO_2 sources are assumed to be distributed over land; the anthropogenic emissions inventories are those developed for St. Louis and the San

TABLE 5. Global nonanthropogenic emissions of various pollutants.

Chemical species	Source strengths kg/y	Distribution
Reactive hydrocarbons	175×10^9	Land (forests)[a]
Nonreactive hydrocarbons	300×10^9	Land[b]
NO_x (exclusive of N_2O)	$1\text{-}100 \times 10^9$	Land or global[c]
SO_2	200×10^9	Land[d]
CO	$1\text{-}5 \times 10^{12}$	Global[e]

[a] Assumes the estimated terpene emissions from Rasmussen et al. (1975) are correct, although some other sources may also be significant.

[b] Assumes the emissions from Rasmussen et al. (1975) for CH_4, although other emissions may be significant.

[c] NO_x minimum corresponds to lightning, maximum corresponds to all sources cited by Rasmussen except N_2O oxidation, a source of nitrate from the stratosphere, but probably not a significant tropospheric NO_x source.

[d] Sum of Rasmussen et al. (1975), SO_2 and H_2S sources. This assumes H_2S oxidation produces 1.9 g SO_2/g H_2S.

[e] CO data from Seiler (1974).

TABLE 6. Anthropogenic and estimated nonanthropogenic emissions for the St. Louis area.

Material	Emissions (kg/yr)		
	St. Louis (RAPS)	S. F. Bay anthropogenic (BAAPCD, 1977)[b]	Natural (Table 5, 1975)[c]
Reactive hydrocarbons (HC1)	5.0×10^7	8.0×10^7	2.0×10^7
Nonreactive hydrocarbons (HC2)	1.8×10^8	2.7×10^8	3.5×10^7
NO_x (as NO_2)	4.8×10^8	2.5×10^8	4.0×10^4 to 2.5×10^7
SO_2	1.2×10^9	8.4×10^7	2.5×10^7
CO	1.5×10^9	1.6×10^9	$0.4\text{-}2 \times 10^8$

[a] 18,603 km^2 area.
[b] 14,400 km^2 of land area, 38,000 km^2 total (includes part of the Pacific Ocean).
[c] 20,000 km^2 area.

Francisco Bay Area. The data in Table 6 imply that, especially for hydrocarbons, biogenic emissions may be a significant component of total emissions even for an urban region. Thus, it would seem desirable to develop methodologies to determine regional biogenic emissions. Measurements of ambient concentrations of various hydrocarbon species do not seem to provide a satisfactory approach because the photochemical lifetimes of some of the more reactive hydrocarbons may be a few minutes, while less reactive hydrocarbons have longer lifetimes. Measurements of emissions from plants and soils in laboratory environments, while not fully satisfactory, seem more promising.

A comparison of the Bay Area and St. Louis emissions inventories reveals substantial differences in patterns (see Table 7). In large part these differences are likely to be real. They reflect differences in population, type of industry, urban geometry, and regulatory environment. However, it is likely that some differences arise as a result of different treatments of raw data, different methods of data acquisition, and different definitions of sources. Some differences seem surprising on first examination, notably the large gross NO_x emissions for St. Louis relative to the San Francisco area. Much of this may reflect more use of coal-fired power plants in the St. Louis area. Table 8 gives areas and population data for four cities for which area source and/or total emissions inventories were available. Table 9 gives per-capita emissions for the various inventories and species. There is still a large range of emissions rates reflected in the various emissions inventories and Table 10 gives emissions per km^2 (land). It is somewhat surprising that the per-capita emissions of hydrocarbons are as high or higher for the California cities with their stricter auto emissions controls than for St. Louis. However, differences in urban

TABLE 7. Gross emissions for various inventories.

Inventory	NO_x kg/day (as NO_2)	Hydrocarbon (kg/day)	CO (kg/day)	SO_2 (kg/day)
St. Louis (RAPS) Total	1.32×10^6	6.38×10^5	4.15×10^6	3.23×10^6
St. Louis (RAPS) Area	3.54×10^5	5.00×10^5	4.06×10^6	3.04×10^4
San Francisco (Eng Div) Total	5.98×10^5	9.06×10^5	3.35×10^6	1.99×10^5
San Francisco (AQMP) Total	6.30×10^5	9.15×10^5	3.87×10^6	2.08×10^5
San Francisco (AQMP) Area	4.56×10^5	7.97×10^5	3.80×10^6	2.90×10^4
Los Angeles Area[a]	1.21×10^6	2.79×10^6	8.59×10^6	—
Denver Area[a,b]	5.91×10^4	1.80×10^5	1.54×10^6	—

[a] Reactive hydrocarbons only.
[b] Omits emission between 2100 and 0500, does not include outer suburbs.

TABLE 8. Approximate population and land area covered by the inventory.

	Area (km^2)	(BEA)[a] 1971 population	Other population	Population adopted
St. Louis	1.86×10^4	3.28×10^6	—	3.28×10^6
San Francisco	1.44×10^4	5.17×10^6	4.76×10^6[b]	4.76×10^6
Los Angeles	4.8×10^4	1.06×10^7	—	1.06×10^7
Denver[c]	2.3×10^3	1.57×10^6	1.26×10^6	1.26×10^6

[a] Bureau of Economic Affairs.
[b] 1975 BAAQMD estimate for Bay Area Pollution Control District.
[c] Denver standard metropolitan statistical area.

geometry may explain most of that. In terms of oxidant, the most noteworthy difference between the various inventories is in the NO_x emissions. On a per-capita basis, the Denver area source emissions of NO_x are about 1/2 the San Francisco Bay Area, St. Louis, or Los Angeles area source emissions, perhaps a reflection of lower atmospheric pressures and/or methodological differences. The per capita RAPS NO_x emissions are about three times larger than for the San Francisco Bay Area. In

TABLE 9. Per capita emissions (kg/person-day).

Inventory	NO_x	HC	CO	SO_2	HC/NO_x (Rates)
St. Louis (RAPS) total	0.402	0.195	1.26	0.98	0.49
St. Louis (RAPS) area	0.107	0.152	1.23	0.009	1.42
San Francisco (Eng Div) total	0.125	0.190	0.70	0.042	1.52
San Francisco (AQMP) total	0.132	0.192	0.81	0.044	1.45
San Francisco (AQMP) area	0.096	0.167	0.79	0.006	1.74
Los Angeles area	0.114	0.263	0.81	—	2.30
Denver area	0.047	0.143	1.22	—	3.04

TABLE 10. Emissions per unit area (kg/km^2 day).

Inventory	NO_x	HC	CO	SO_2
St. Louis (RAPS) total	71.0	34.3	242	174.
St. Louis (RAPS) area	19.0	26.9	218	1.6
San Francisco (Eng. Div.) total	41.5	62.9	233	13.8
San Francisco (AQMP) total	43.7	63.5	269	14.4
San Francisco (AQMP) area	31.7	55.3	264	2.0
Los Angeles area	25.2	58.1	179	—
Denver area	25.7	78.2	669	—

large part this reflects the several major coal-fired power plants in the St. Louis area, as do differences in the SO_2 emissions.

In terms of model performance evaluation, it will be worth remembering that in St. Louis, unlike the Bay Area, one of the pollutants (NO_x) important in oxidant formation is dominated by elevated point source emissions. As a result, the treatment of elevated emissions can potentially create large errors in model performance in the St. Louis area, errors not likely to be of comparable importance in the San Francisco Bay Area.

Indeed, we will find that we tend to underpredict ozone in St. Louis, and so do most other models applied to St. Louis (J. Shreffler, P. Roth, private communications, 1979). There are two plausible reasons for this that relate to emissions inventories. One is that significant biogenic hydrocarbon emissions are not reflected in the RAPS inventory. The other is that perhaps elevated NO_x and SO_2 emission sources should be excluded unless the mixing depth is substantially deeper than 100 m since the major power plant plumes should rise to higher levels.

SECTION 5

ANALYSIS OF METEOROLOGICAL DATA

The LIRAQ models require mass-consistent flux fields and optical transmissivity fields consistent with the grid structure of the model. The MASCON code (MacCracken et al., 1978; Dickerson, 1973, 1978; Stullich et al., 1978) has been developed to generate these fields for the LIRAQ models.

To drive MASCON, one must provide topographic information (see Section 7), wind measurements, mixing depths, and solar-flux measurements. For this study we have developed processors that generate MASCON input files from RAMS data tapes combined with subjectively developed mixing depths. These processors are described in Appendices C-F.

Here, we emphasize that methods other than MASCON for generating mass-consistent flux fields have been developed by others and might well be used by LIRAQ. Similarly, the estimation of mixing depths involves subjective decisions that no two qualified analysts would always agree on.

When models are compared, we would suggest that the subjective methodologies involved in generating model input be kept as constant as possible.

SECTION 6

PHOTOCHEMICAL SUBMODEL

The LIRAQ photochemical submodel is designed to reproduce the homogeneous inorganic chemistry of smog formation in as much detail as is feasible using the best available measurements for reaction-rate constants or estimates for the reaction-rate constants when appropriate measurements do not exist. The submodel is designed to approximate organic reaction rates using a lumping scheme for organic species similar to that proposed by Hecht et al. (1974) but using a modified set of reactions and rate coefficients. As a result of the lumping procedure, the organic species we use are not real, chemically identifiable molecules, but a kind of "average" molecule. As such, their rates of reaction and molecular weights are not those of any real compound and cannot be directly determined, except by averaging measured or estimated rates of the various compounds associated with the lumped species.

The reasons for adopting this structure for the photochemical model are discussed in this section along with a more detailed description of the rate constants and of the procedures used in the formulation of the submodel and in the generation of the rate constants. We present the validation/tuning of the submodel and a discussion of the recent changes in the LIRAQ-2S model along with a brief discussion of some model sensitivities.

We decided to lump organic species because of computational restraints, limitations in our knowledge of reaction mechanisms and rate data, and uncertainty in the detailed breakdown of the organic emissions inventory. The storage capacity of computers is limited, and an attempt to explicitly include all organic compounds in gasoline, auto exhaust, aviation fuels, solvents, refinery emissions, and the products and reactive intermediates produced by these chemicals as a result of photochemical reactions would involve at least several hundred or possibly several thousand chemically distinct compounds. Even a one-box simulation of a complete and detailed photochemistry would be difficult to compute. This would be true even if the necessary rate and source data existed; however, those data are largely nonexistent.

Several of the reactions assumed in the organic reaction set have never been measured for any species; most have only been measured for a few of the simplest compounds in the class. In several situations, the relevant rates have only been measured for the one-carbon atom compound in the class. In most situations, this compound is likely to be the least-typical member of that class. More important than the lack of rate data are the several uncertainties in the mechanistic structure. The rate constant for the reaction of ozone with alkenes has been measured for several compounds, but with the exception of ethene, probably the least typical alkene, the products of the reaction (at least under atmospheric conditions) are poorly known. Several other reactions are subject to similar uncertainty including such major reactions as the reaction of peroxyacyl radicals with nitric oxide and the reaction of oxygen atoms with alkenes.

Of equal importance is the uncertainty in the emissions inventory. Gasoline composition varies from year to year and company to company. Automobile exhaust composition can be assumed to be a function of the automobile, the gasoline, and the mode of operation. Extensive but incomplete analyses of both are available. However, the agreement between analyses by different agencies is far from perfect and the actual emissions are only approximately known. For nonautomotive sources, much fewer data are available. An attempt to incorporate the information derived by Trijonis and Arledge (1975) for Los Angeles in the San Francisco Bay Area emissions inventory is described in Appendix B of Duewer et al. (1978).

As demonstrated above, the model is forced to use a simplified organic reaction mechanism. Given this, it seems reasonable to generate a simulation model in which the reaction mechanism would be arbitrary and the rate coefficients would be free parameters. If adequate data existed for the tuning of such a model, this would be the best method for many applications. However, adequate data do not exist, and are unlikely to be generated in the near future because the potentially large number of free parameters implied by such a model introduces many degrees of freedom that must be tied down.

To reduce the number of parameters and make maximum use of laboratory data, it was decided to use a chemical reaction set that explicitly includes most of the important inorganic species and reactions, but that uses composite (lumped) species to represent the organic molecules and uses a greatly simplified set of reactions of organic molecules and products. This should provide the best representation of well-known physical processes consonant with computational limitations, the overall structure of the model, and available data. The goal was a model with few dynamically calculated species, but with many structural similarities to the more complex mechanism the model is designed to simulate, and with a minimum of free parameters. The omission of a reaction is equivalent to setting the rate constant to zero, which is often less justifiable than using another value, even when the actual rate may not be exactly known.

Because most of the inorganic reaction products and rate coefficients are known with some degree of precision, these reactions and rate coefficients were adopted from the literature as of mid-1976. Although substantial uncertainties exist about some of these processes, the best literature value available at that time was adopted and, except for new data, no tuning of the inorganic reaction set was permitted. Because the model neglects some possible reactions, accurate values for the known reaction rate coefficients might well not lead to the most accurate model. However, use of the best measured rate coefficients isolates the free parameters, should allow correction, transfer, or elaboration of the model more easily, and is intuitively easier to justify than some other set of coefficients.

The fairly complex organic reaction mechanism was chosen to include as many as is feasible of the types of reactions to be anticipated in atmospheric smog formation. Further, although the organic reaction rates are parameters and are designed to include neglected parallel processes, the ranges of reaction rate coefficients considered were limited to those plausible for the classes of reaction considered. They are tuned within this range to improve the agreement between computed smog chamber behavior and experience. Although we used these criteria for choosing the reaction rate coefficients, they should not be accepted as either correct or optimal. We chose them to generate a reaction mechanism that can be amended with a minimum of retuning and that can be intuitively defended. A better fit to smog chamber data could be made if more rates were to be treated as parameters. Better agreement with smog chamber and atmospheric behavior would be expected if more chemical species or reactions were to be included. However, the smog-chamber data include processes not expected in the atmosphere, and additional complexity in the mechanism to be used in a regional model is undesirable because it costs computer time, because excessive complexity invites coding errors, and because more free parameters are introduced. The mechanism given in Table 11 includes several different types of approximations inherent in the general form.

The choice of hydrocarbon classes was governed by the considerations given by Hecht et al. (1974); that is, species reacting with the same set of species are grouped together. The definitions of the species are as follows. HC1 reacts with oxygen atom, ozone, and hydroxyl radical (roughly equivalent to alkenes and reactive aromatic compounds); HC2 reacts with oxygen atom and hydroxyl radical (alkanes, some ketones, less-reactive aromatic compounds, many alkyl halides, etc.); HC4 is photolysed, reacts with hydroxyl radicals, and oxygen atoms, and reacts slowly with peroxy radicals and NO_3 (aldehydes, some aromatic compounds, some ketones, etc.). Hecht et al., also used class HC3, which represented aromatic compounds (not included in Hecht's HC2 class). However, in their mechanism, HC2 and HC3 unrealistically undergo identical reactions at similar rates; thus, the distinction is not preserved in this model. (More recent studies of aromatic molecules at Systems Analysis, Inc., SAI, e.g., Whitten and Hogo (1977) have a more realistic representation of the role of aromatic molecules.) RO symbolizes alkoxyl radicals, RO_2 symbolizes alkyl proxyl radicals. ROOH is an organic hydroperoxide, RNO_2 an organic nitrite, RNO_3 an organic nitrate, and PAN a peroxyacyl nitrate. All other species are indicated by conventional chemical formulae.

The lumping of many similar chemical species into one average species results in a set of rate coefficients that only approximately describe the reactions of the individual compounds in the class. If a wide range of rate coefficients is involved (as for OH and alkanes, less reactive aromatic compounds and ketones (HC2)), then the value of the average rate coefficient would be a function of time. If different compounds within a class produce products in different classes (e.g., the photolysis of aldehydes) then both average rate constants and products are defined only in an average sense and the correct average for atmospheric use is difficult to estimate because the inventory is poorly known.

In addition to the above approximations inherent to lumping, there are several other mechanistic approximations. Some reactions produce products omitted from the model that rapidly lead to other products that are used. An example is

$$OH + CO \rightarrow H + CO_2, \qquad H + O_2 \xrightarrow{M} HO_2.$$

Because H has no other known reactions significant in the troposphere, this sequence is treated as

$$OH + CO \rightarrow CO_2 + HO_2.$$

TABLE 11. Reactions of the photochemical submodel.

Reaction No./Footnote	Reaction	A,cm-s[a]	C, K[a]
	Photolysis		
Q40[b,c]	$O_3 + h\nu \rightarrow O + O_2$		
Q42[b,c,d]	$O_3 + h\nu \xrightarrow{H_2O} O_2 + 2OH$		
Q1[b,c]	$NO_2 + h\nu \rightarrow NO + O$		
Q37[e,b,f]	$NO_3 + h\nu \rightarrow NO_2 + O$		
Q12[g,b,f]	$HNO_2 + h\nu \rightarrow HO + NO$		
Q17[b,c,h]	$H_2O_2 + h\nu \rightarrow 2OH$		
Q23[b,c,i]	$HC_4 + h\nu \rightarrow RCO_3 + HO_2$		
Q51[b,c,i]	$HC_4 + h\nu \rightarrow CO + H_2$		
	O_x-NO_x-HO_x Reactions		
Q2[j]	$O + O_2 + M \rightarrow O_3 + M$	1.07×10^{-34}	510
Q3[j,k]	$O_3 + NO \rightarrow O_2 + NO_2$	1.0×10^{-12}	-1200
Q4[j]	$O + NO + M \rightarrow NO_2 + M$	4.0×10^{-33}	940
Q5[j]	$O + NO_2 \rightarrow NO + O_2$	9.1×10^{-12}	0
Q6[j,k,l]	$O + NO_2 + ZM \rightarrow NO_3 + ZM$	3.5×10^{-12}	300
Q7[j,k]	$O_3 + NO_2 \rightarrow NO_3 + O_2$	1.1×10^{-13}	-2450
Q8[m]	$NO_2 + NO_3 \rightarrow N_2O_5$	3.8×10^{-12}	0
Q9[m]	$N_2O_5 \rightarrow NO_2 + NO_3$	$5.7 \times 10^{+14}$	-10600
Q10[j]	$NO + NO_3 \rightarrow 2NO_2$	8.7×10^{-12}	0
Q11[n]	$N_2O_5 + H_2O \rightarrow 2HNO_3$	3.0×10^{-16}	-3300
Q13[o]	$HO + NO_2 \xrightarrow{M} HNO_3$	1.0×10^{-11}	0
Q14[g]	$HO + NO \xrightarrow{M} HNO_2$	6.0×10^{-12}	0
Q15[j]	$HO + CO \rightarrow CO_2 + HO_2$	1.4×10^{-13}	0
Q16[n]	$HO_2 + NO \rightarrow HO + NO_2$	1.0×10^{-11}	-350
Q46[p]	$HO + HO_2 \rightarrow H_2O + O_2$	2.0×10^{-11}	0
Q44[q]	$HO_2 + NO_2 \rightarrow HNO_4$	2.0×10^{-14}	0
Q48[n]	$HO_2 + O_3 \rightarrow HO + 2O_2$	6.0×10^{-14}	-1220
Q52[j]	$HO + O_3 \rightarrow HO_2 + O_2$	1.6×10^{-12}	-1000
Q50[r]	$HO + HNO_3 \rightarrow H_2O + NO_3$	9.0×10^{-14}	0
Q31[s]	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	1.7×10^{-11}	-500

TABLE 11. Continued.

Reaction No./Footnote	Reaction	A,cm-s^a	C, K^a
	Reactions of HC1		
Q18[j,l,t]	$HC_1 + O \rightarrow RO_2 + RCO_3$	1.0×10^{-11}	-360
Q19[j,t]	$HC_1 + O_3 \rightarrow HO_2 + RO + HC_4$	7.0×10^{-15}	-1900
Q20[u,t]	$HC_1 + HO \rightarrow RO_2 + HC_4$	4.0×10^{-11}	-120
Q49[u,t]	$HC_1 + HO \rightarrow RO_2 + H_2O$	3.0×10^{-11}	-350
Q54[v,t,w]	$HC_1 + NO_3 \rightarrow NO_2 + HC_2$	5.0×10^{-13}	-1400
Q57[v,t,w]	$HC_1 + HO_2 \rightarrow HO + HC_2$	0	0
	Reactions of HC2		
Q21[x,t]	$HC_2 + O \rightarrow RO_2 + HO$	3.2×10^{-11}	-2000
Q22[x,t]	$HC_2 + HO \rightarrow RO_2 + H_2O$	4.5×10^{-11}	-900
	Reactions of HC4		
Q24[j,t]	$HC_4 + HO \rightarrow RCO_3 + H_2O$	1.5×10^{-11}	-350
Q34[j,t]	$HC_4 + O \rightarrow HO + RCO_3$	3.2×10^{-12}	-900
Q38[j,t]	$HC_4 + HO_2 \rightarrow H_2O_2 + RCO_3$	8.0×10^{-13}	-3700
Q47[j,t]	$HC_4 + HO \rightarrow CO + HO_2 + H_2O$	3.0×10^{-11}	-350
Q45[v,t,w]	$HC_4 + NO_3 \rightarrow RCO_3 + HNO_3$	3.0×10^{-15}	-900
Q39[v,t,w,y]	$HC_4 + RO_2 \rightarrow ROOH + RCO_3$	8.0×10^{-13}	-3750
	Reactions of SO_2		
Q41[m]	$HO_2 + SO_2 \rightarrow HO + SO_4^=$	5.0×10^{-18}	0
Q32[j]	$HO + SO_2 \rightarrow HO_2 + SO_4^=$	6.0×10^{-13}	0
Q43[v,y]	$RO + SO_2 \rightarrow HO_2 + SO_4^=$	4.0×10^{-13}	0
Q35[v,y]	$RO_2 + SO_2 \rightarrow RO + SO_4^=$	2.0×10^{-18}	0
Q56[v,y]	$RCO_3 + SO_2 \rightarrow RO_2 + SO_4^= + CO_2$	1.0×10^{-19}	0
	Organic radical reactions		
Q53[v,y]	$RCO_3 + RCO_3 \rightarrow HC_4 + CO_2$	1.0×10^{-12}	0
Q25[g,y]	$RO_2 + NO \rightarrow RO + NO_2$	4.0×10^{-12}	-300
Q26[v,y]	$RCO_3 + NO \rightarrow RO_2 + NO_2 + CO_2$	3.0×10^{-12}	-300
Q27[v,y]	$RCO_3 + NO_2 \rightarrow PAN$	2.7×10^{-13}	0

TABLE 11. Continued.

Reaction No./Footnote	Reaction	A,cm-s[a]	C, K[a]
Q28[z,g,y]	$RO + O_2 \rightarrow HO_2 + HC_4$	1.0×10^{-12}	-2200
Q29[v,y]	$RO + NO_2 \rightarrow RNO_3$	2.0×10^{-12}	0
Q30[v,y]	$RO + NO \rightarrow RNO_2$	2.0×10^{-12}	0
Q36[v,y]	$RO_2 + HO_2 \rightarrow ROOH + O_2$	2.7×10^{-12}	0
Q33[v,y]	$RO_2 + RO_2 \rightarrow RO + RO + O_2$	2.7×10^{-13}	0

[a] A and C defined by K + A exp(C/T), where T is temperature in K.

[b] All photolysis rates are calculated as a function of solar zenith angle.

[c] M. C. MacCracken and G. D. Sauter, "Development of an Air Pollution Model for the San Francisco Bay Area," Lawrence Livermore Laboratory, Report UCRL-51920, Vol. 2 (1975).

[d] The rate used assumes the fate of $O(^1D)$ is either reaction with water or quenching by N_2 or O_2, and that the water concentration is $2.4 \times 10^{17}/cm^3$.

[e] Harold Johnston, Lawrence Berkeley Laboratory, Berkeley, California, private communication (1975).

[f] The products and quantum yields for NO_3 photolysis have recently been remeasured. We expect to revise the mechanism accordingly. (About 30% of the photolysis should yield $NO + O_2$.)

[g] G. Z. Whitten and H. Hogo, "Mathematical Modeling of Simulated Photochemical Smot," U. S. Environmental Protection Agency, Office of Research and Development, Research Triangle Park, North Carolina, Report 600/3-77-0111 (1977).

[h] Recent measurements indicate that the photolysis of H_2O_2 in the troposphere should be significantly faster than our current treatment has it.

[i] There is reason to believe that the quantum yields for aldehyde photolysis may be pressure dependent and substantially less than one.

[j] R. F. Hampson and D. Garvin, "Chemical Kinetics and Photochemical Data for Modeling Atmospheric Chemistry," National Bureau of Standards, Washington, D. C. Technical Note 866 (1976).

[k] This rate constant has been rounded and a small difference exists between the referenced review and our treatment.

[l] Temperature dependence has been assumed.

[m] D. L. Baulch, D. D. Drysdale, D. G. Horne and A. C. Lloyd, "Evaluated Kinetic Data for High Temperature Reactions, V. 2 Homogeneous Reactions of the H_2-N_2-O_2 System," (Butterworths Ltd., London, 1977).

[n] An estimate based on an attempt to reconcile conflicting data.

[o] J. Anastasi and I. W. M. Smith, "Kinetics of the Reaction $OH + NO_2 (+ M) \rightarrow HNO_3 (+ M)$ Over a Wide Range of Temperature and Pressure," *J. Chem. Soc., Faraday Trans.*, *172*, 1459 (1976).

[p] An estimate based on upper limit data cited by F. Kaufman, University of Pittsburgh, and C. J. Howard, NOAA, Boulder, in separate private communications (1977).

[q] This represents an attempt to come to terms with an apparent fast rate of formation for HNO_4 ($\sim 2 \times 10^{-12}$ in the lower troposphere), a short but poorly known lifetime for HNO_4 vs. unimolecular decay ($\sim$1-10 s), and probable efficient scavenging of HNO_4 on surfaces).

[r] R. Zellner and I. W. M. Smith, "Rate Constants for the Reactions of OH with NH_3 and HNO_3," *Chem. Phys. Letters*, *26*, 72 (1974).

[s] A. C. Lloyd, "Evaluated and Estimated Kinetic Data for Gas Phase Reactions of the Hydroperoxyl Radical," *Intern. J. Chem. Kinet.*, *6*, 169 (1974).

[t] Reaction rate constants based on reference compound propene for HC1, butane for HC2, and average of methanal and ethanal for HC4.

[u] D. D. Davis, Georgia Tech. University, private communication (1976).

[v] Estimated from model and fit to chamber data.

[w] A rough estimate based on little data. Rate constant is chosen to be small enough not to have a major effect on simulations.

[x] Estimate based on a room temperature rate from Hampson and Garvin (1976) and an assumed temperature dependence.

[y] There is little reliable quantitative data pertinent to the rate of any reaction of organic free radicals important smog chemistry, and because the radicals used in LIRAQ are generalized radicals rather than specific chemical species, it is not conceptually possible to develop correct rates for these reactions in a model of this sort. Rates used are derived from simulations of smog chambers or are estimated from similar reactions.

[z] J. R. Barker, S. W. Benson, and D. M. Golden, "The Decomposition of Dimethyl Peroxide and the Rate Constant for $CH_3O + O_2 \rightarrow CH_2 + HO_2$," SRI Project 2294, SRI, International, Menlo Park, CA (1976).

Another type of approximation is involved in our treatment of peroxy nitric (HNO_4) acid formation. We assume a fast equilibriation between formation and loss of HNO_4 with a slower heterogeneous loss of HNO_4. We do not compute HNO_4 explicitly, but use a slow formation rate designed to simulate heterogeneous loss of NO_x as HNO_4. Many reactions are omitted, some because their inclusion has no significant effect on the predictions of the model. Examples would be the reactions

$$OH + OH \rightarrow H_2O + O, \qquad O_3 + HC2 \rightarrow \text{products}.$$

Others are omitted because they would complicate the mechanism and are not sufficiently well-established for their effects to be assessed. Examples are

$$OH + PAN \rightarrow \text{products}$$

and

$$RCO_3 + HC1 \rightarrow \text{products},$$

where PAN is a peroxyacyl nitrate. Important reactions may be omitted because their existence is not suspected.

By comparing the predictions of lumped models with detailed models and experiments, the effects of lumping could be assessed if detailed (unlumped) reaction systems had been experimentally examined in sufficient detail and a full set of reaction rates were available. The available data are not sufficient to permit such a test, although this may change. The effects of deliberate omissions or use of composite reactions can be assessed by making calculations including the omitted reactions or the explicit detailed form of the reaction. This has been done as a test of the effect of these approximations.

The effect of omitted reactions with unknown rates or products or the effects of unsuspected reactions cannot be assessed. For some reactions, especially some radical recombination reactions, other parallel radical-loss mechanisms are effectively incorporated in the set. Thus, the rate coefficients derived from tuning against smog chamber data are not those that would be measured in the laboratory, even if averaged. Because the operating parameters of smog chambers differ from those usually encountered in the atmosphere in temperature, solar flux, and spectral distribution, concentration and identity of reactive species, and surface-to-volume ratio, the tuning of the parametric rates against chamber data is theoretically unsatisfactory. Nevertheless, it seems the best available approach. In the future, atmospheric data could possibly be used in a trajectory model to provide an alternative tuning system, but at present, no atmospheric data base exists that is adequate for that purpose.

Reactions Q1-17 in Table 11 are mechanistically well established, and their rates are experimentally based, although the rate of reaction Q15 may be pressure-dependent and should probably be increased by a factor between 1.1 and 2 for tropospheric conditions. These reactions should be adjusted in mechanism or rate only if new kinetic data require it. The reactions of stable hydrocarbon species can be described as follows. The rates should all be functions of the composition of the initial charge or emissions, those dealing with the reactions of HC4 (aldehydes), should be functions of all other reaction conditions and time. Mechanistic approximations are made in the reactions of HC1 with O and O_3, which are thought to produce ketones for some alkenes. The direct products may include Crigee zwitterions and various ozonosides and ozonides, only some of which will lead to the products we consider. Reactions of HC4 (aldehydes) should often lead to RO_2 or RCO_3, if the aldehyde is not formaldehyde, and to HO_2 if the aldehyde is formaldehyde. In some cases, only one of these sets of products has been included in the mechanism.

Reactions of organic free radicals generally have poorly established rates. Almost no reliable data are available for radicals other than those derived from methane. What is available, even for the one-carbon-atom compound, is usually based on indirect measurements or on measurements of complex reaction mixtures. The rate coefficients initially used are largely based on "chemical intuition" and some are tuned over the full order of magnitude we allowed. This group of reactions could almost certainly be expanded with an improvement in expected fit if reliable values were used. The paucity of persuasive data to guide the selection of rate coefficients (and reaction products) has discouraged this.

In chamber simulations, we have adopted the values used by the experimenters or by other modelers for photolysis reactions. In modeling the atmosphere, we calculate the rates from the cross-section and the calculated solar flux. Reaction Q42 is a lumping of the rate-limiting production of $O(^1D)$ from ozone photolysis and the competing $O(^1D)$ destroying processes

$$O(^1D) + H_2O \rightarrow 2OH,$$

and

$$O(^1D) + ZM \rightarrow O + ZM.$$

A water density of $2.46 \times 10^{17}/cm^3$ is implicit in the rate coefficient used for Q42.

Rate-constant errors are likely to lead to errors smaller than mechanism errors, and the most serious deficiency in the mechanism may be the processes omitted. The most obvious of these omissions are the decomposition of PAN and HNO_4 and reactions of such species as PAN, RNO_2, ROOH, RNO_3 and HNO_2 with OH, O, and the peroxyl radicals. All of these chemical species should be at least as reactive as HC2. The reactions of some of the above species might be important sources of NO and NO_2 at times after the NO_2 peak.

Many radical reactions have been omitted. However, unless the rate constants are substantially larger than seems plausible, or the free radical concentrations higher than predicted in the model, most of these reactions can have little effect on the course of oxidant generation. Exceptions to the above might be the reactions

$$RCO_3 + RO_2 \rightarrow \text{products}$$

and

$$RCO_3 + HO_2 \rightarrow \text{products}.$$

If the products include OH or lead to the net destruction of two radicals, those reactions could be important, especially after the ozone peak.

SULFUR CHEMISTRY

To treat the homogeneous conversion of SO_2 to sulphate, the following nonstoichiometric reactions from Table 11 have been included in the mechanism:

$$OH + SO_2 \xrightarrow[O_2,H_2O]{} SO_4^{=} + HO_2 \qquad (Q32)$$

$(k = 6 \times 20^{-13})$,

$$HO_2 + SO_2 \xrightarrow[H_2O,M]{} SO_4^{=} + HO \qquad (Q41)$$

$(k = 5 \times 10^{-18})$,

$$RO_2 + SO_2 \xrightarrow[H_2O,M]{} SO_4^{=} + RO \qquad (Q35)$$

$(k = 2 \times 10^{-18})$,

$$RO + SO_2 \xrightarrow[H_2O,M]{} SO_4^{=} + HO_2 \qquad (Q43)$$

$(k = 4 \times 10^{-13})$,

and

$$RCO_3 + SO_2 \xrightarrow[H_2O,M]{} SO_4^{=} + RO_2 + CO_2 \qquad (Q56)$$

$(k = 1 \times 10^{-19})$.

The rate constant used for Q41 above is based on measurements and data cited by Hampson and Garvin (1975). The rate constant used for Q32 reflects privately communicated data from J. Calvert (1977). The rate constants for Q35, 43 and 56 are estimates based on the rate constants for Q41 and Q32 and the assumption that the activation energy is about 2 kcal less for reaction with RO_2 or RCO_3 than the reaction with HO_2. Thus, these rate coefficients are speculative. In simulations of Bay Area air quality, reaction Q41 dominates SO_2 conversion. SO_2 oxidation has little effect on O_3 or radical concentrations computed by LIRAQ.

In addition to the above reactions, reconsideration of the behavior of chamber simulations and recently published experimental data led us to revise the basic mechanism extensively. The revised chemistry is included in Table 11. This revision dates from the spring of 1976. A further revision will be done in the early part of 1980.

TUNING OF THE MODEL

Because the data were easily available and some of the tuning had already been done by Hecht et al. for their similar model, the parametric variables were initially coarsely tuned against the EPA smog-chamber data used by Hecht. The nonparametric rates were not tuned, and the parametric rates were tuned within a reasonable range. No effort was made to fit the EPA data precisely, but consistent discrepancies were examined and an effort was made to correct them.

The model does consistently fail to produce as much O_3 as the EPA chamber at high initial alkene and NO concentrations. With less-reactive hydrocarbon systems, the model is more faithful. The overall fit to the EPA data is slightly worse than that obtained by Hecht, better for some simulations, worse for others. This level of agreement is a deficiency for the LIRAQ-2S photochemical model relative to the model of Hecht, because our model is significantly more complicated than their model. However, this failure is not as serious as it would be if our model were a pure simulation model, because we made less effort to fit the smog chamber data than did Hecht, and we made more effort to preserve the physical content of the rate constants used in nonparametric reactions. This decision seems justified because of the behavior of the model in simulations of U. C. Riverside data.

STUDIES USING U. C. RIVERSIDE DATA

Verification studies have been made using this reaction set and U. C. Riverside data presented in Whitten and Hogo (1977). Like them, we find that our reaction mechanism does not generate enough O_3 rapidly enough, unless an additional radical source is postulated. Also, as these authors found, we find that if we assume HNO_2 to be initially present at concentrations of 0.1-10 ppb, we can fit the U. C. Riverside data well. Sample simulations are presented in Figure 2.

At best, it is speculative to assume ppb levels of initial HNO_2. Thus, the simulations using such levels of HNO_2 should not be viewed as lending confidence to the present mechanism; rather, those simulations suggest that the chamber contains an unknown source of free radicals that is either (1) an initial impurity, perhaps HNO_2, (2) an unsuspected chemical mechanism, or (3) a chamber artifact. All three explanations are plausible. Heterogeneous formation of HNO_2 during gas handling is suggested by Whitten and Hogo and may be significant. Only optimistically could one claim to fully understand the mechanisms of smog formation. Chamber artifacts are by no means impossible, even given the great care taken by the Riverside group, which inspires us to feel more confidence in their results than in the results of most other smog chamber research. The sensitivity of the revised mechanism to temperature, humidity, and light intensity is indicated in Figures 3 through 5. Like the earlier LIRAQ mechanism, the revised mechanism is sensitive to light intensity, insensitive to humidity, and moderately sensitive to temperature. Like the old mechanism, the new LIRAQ model predicts slower O_3 formation, but a higher O_3 maximum if the temperature is lowered. The higher O_3 maximum at lower temperatures is largely a response to the activation energy of the reaction

$$NO + O_3 \rightarrow NO_2 + O_2 \quad ,$$

while the slower rate of formation is a response to the activation energy associated with initiation reactions. If heterogeneous processes are important in producing HNO_2, or if there are significant (especially negative) activation energies associated with radical termination reactions, the temperature sensitivity could be significantly incorrect.

NEED FOR FURTHER WORK

In the three years since the revised LIRAQ-2S reaction set was prepared, several new laboratory measurements have appeared in the literature. As a result of these, it is likely that changes should be made in the treatment of O_3, HC_4, NO_3, and H_2O_2 photolysis. Changes should also be made in the rates of most reactions (most notably the reactions of HO_2 + NO, HO_2 + O_3, and several reactions involving RO_2 or RCO_3). Also, the products of some reactions involving RCO_3 might be changed, and reactions of PAN should be added if multi-day simulations are desired.

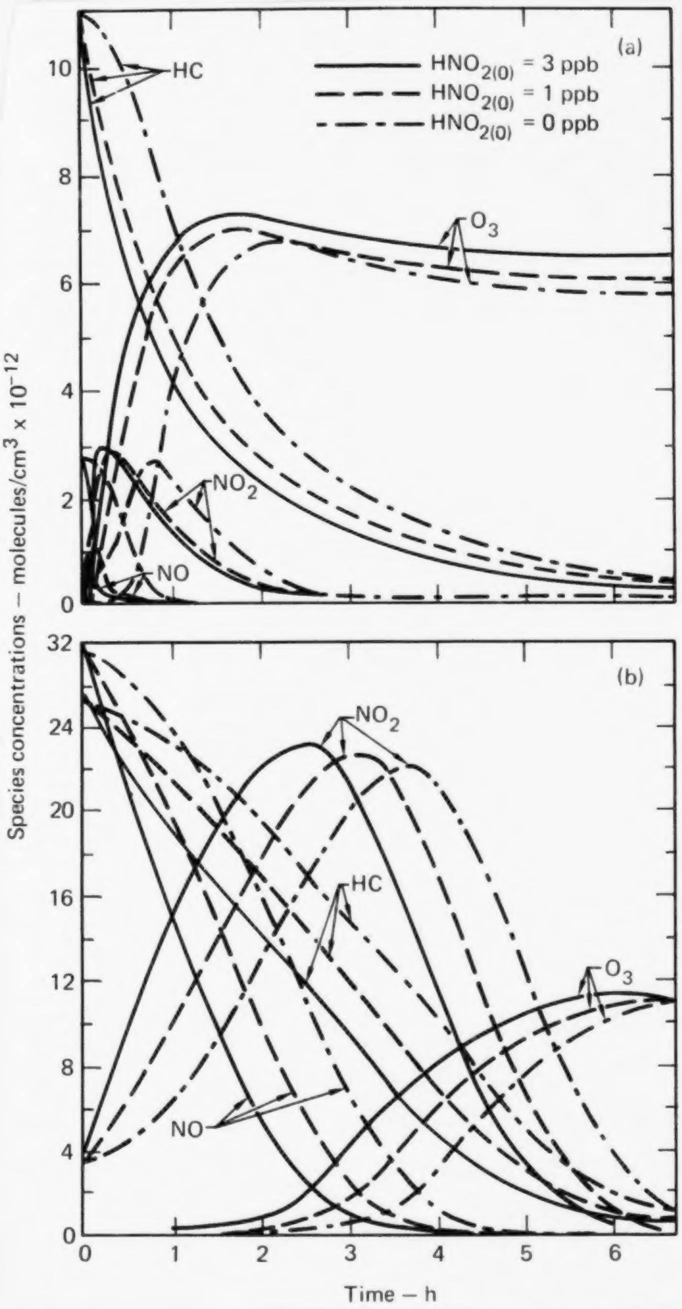

FIGURE 2. Simulation of University of California Riverside run EC-11 (a) and EC-16 (b) for three initial concentrations of nitrous acid.

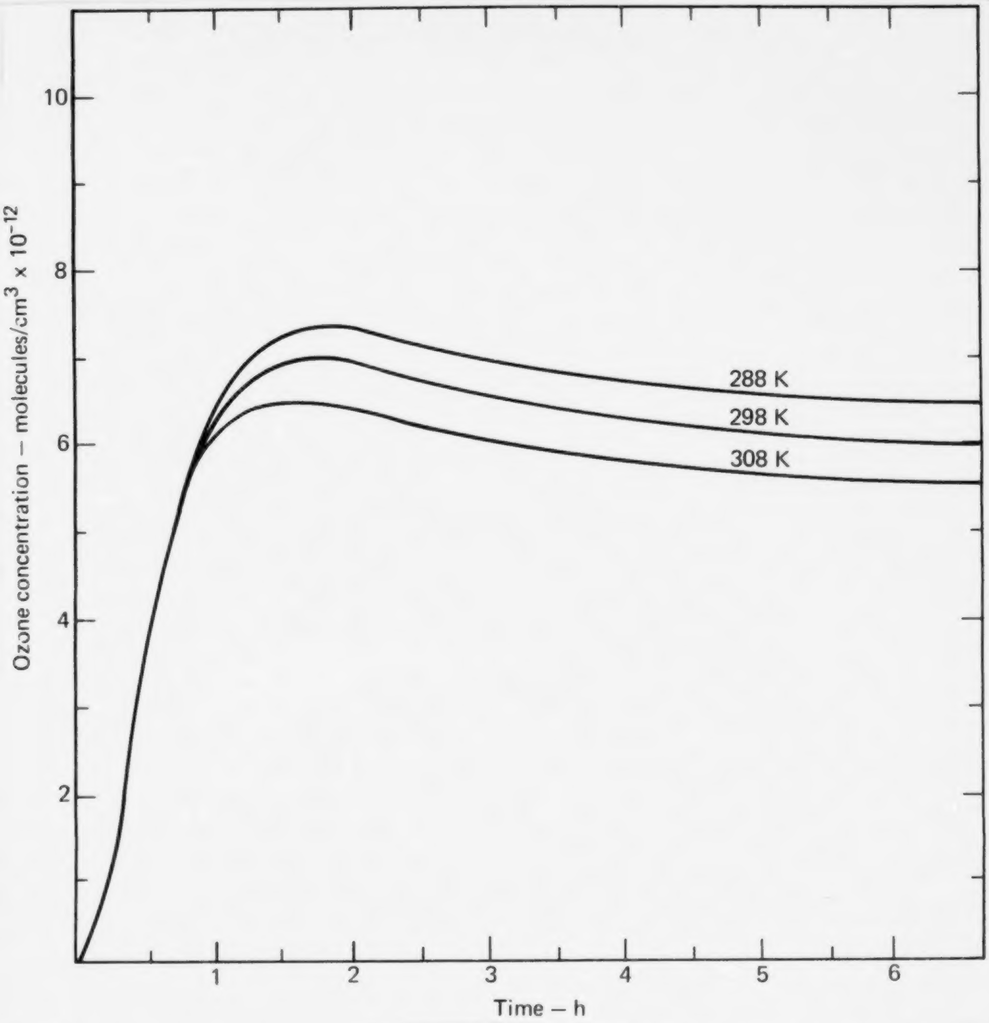

FIGURE 3. Model predicted O_3 concentration vs. time for three temperatures. All other parameters held constant.

Because LIRAQ lacks vertical resolution, it is not particularly good for studying SO_2 and sulphate. If a more economical version of LIRAQ-2S were desired for use in studying O_3, it would then be feasible to remove HNO_3, SO_2, and $SO_4^=$ from the model and add PAN. The resulting model should cost about 40% less to run than the existing model. (Alternatively, the number of grid elements might be increased to about 25 x 25).

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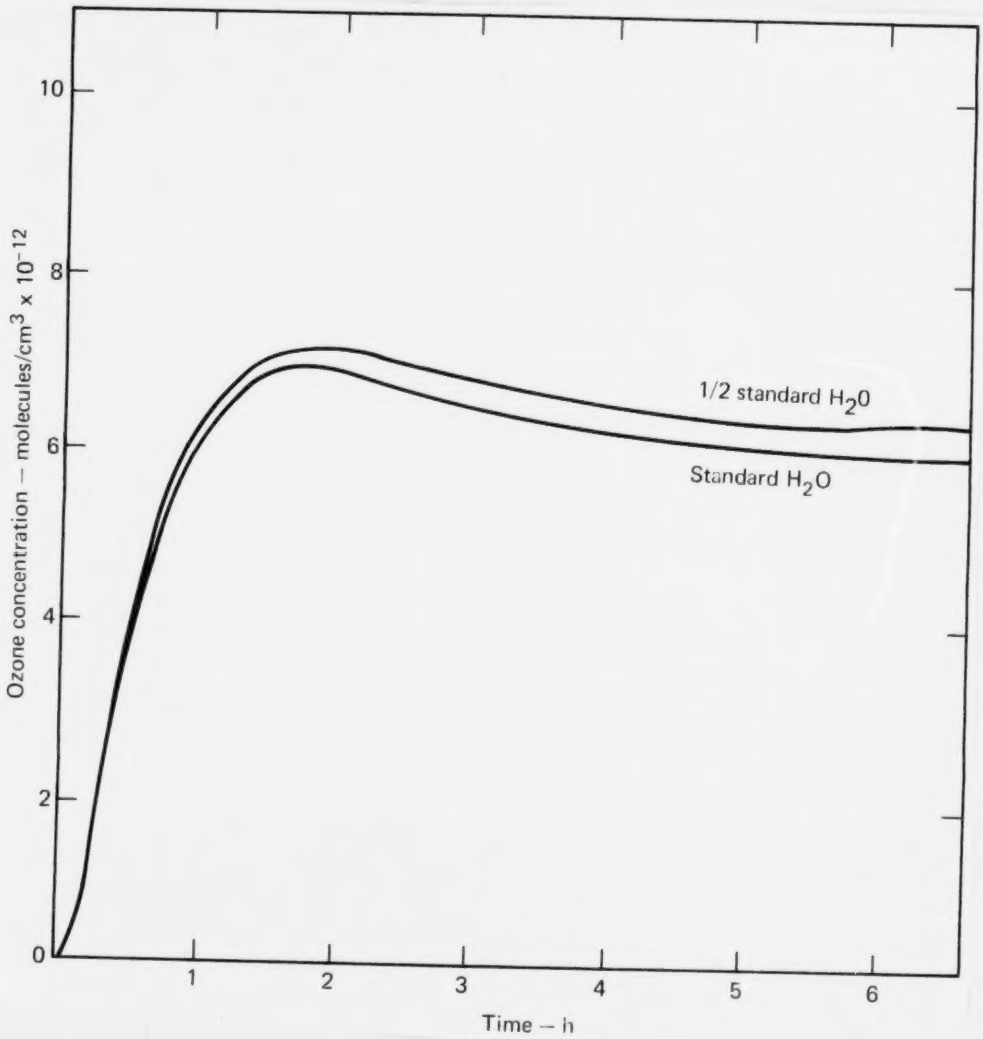

FIGURE 4. Model predicted O_3 concentrations vs. time for two absolute water vapor concentrations. All other parameters held constant.

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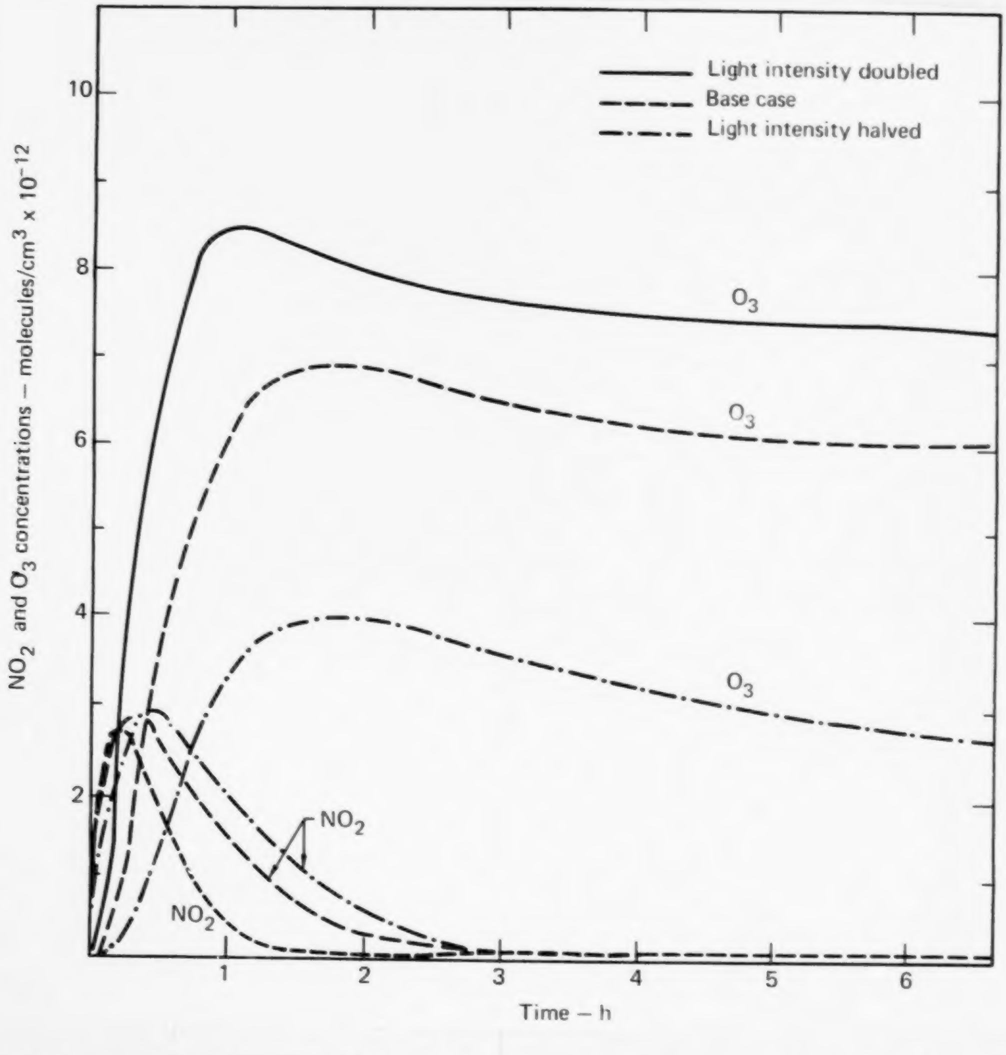

FIGURE 5. Model predicted O$_3$ and NO$_2$ concentrations vs. time for three light intensities. All other parameters held constant.

SECTION 7

TOPOGRAPHIC DATA

The QGEO file contains information on air monitoring stations, river and other map outline segments, and topography. Each of these categories constitutes one of the three data sections of the QGEO file; each section is delimited by a unique and recognizable header card. A comment section describing the QGEO file format precedes the data section.

The station section contains air-monitoring station definitions and a list of stations to plot on graphical output frames. A station is defined by assigning to it a plotting symbol and number, and by specifying its UTM (Universal Transverse Mercator) projection coordinates. To avoid overcrowding on graphical output frames, a separate list is maintained of stations that have their symbols plotted at the corresponding station locations.

To aid the user in identifying locations on the model grid, the MASCON and LIRAQ models allow up to 25 curve segments to be plotted on the graphical output frames. Each curve segment is defined by a list of UTM easting-northing coordinate pairs that are plotted as a continuous curve. No more than 1000 points may be used in defining all segments. This feature may be used to plot river, shoreline, or political-boundary segments.

The MASCON model requires topographic data to derive realistic mass-consistent flow patterns through its adjustment process. The vertical distance between topography and the overlying inversion base determines the type and position of internal boundaries across which the flow of air (and pollutants) is restricted.

Topographic data for the St. Louis region were taken from digital terrain files of the United States Geological Survey's National Cartographic Information Center. The data in these files were obtained by digitization of 1:125,000 scale map sheets using a 0.01-in. grid (approximately 60 m full scale). For use in a QGEO file, the data were extensively thinned and projected onto a 1-km UTM grid.

When running a MASCON or LIRAQ model using a 1-km grid interval, we used all topographic points in the QGEO file. For model runs with a larger grid interval, we selected points at grid intersections (without averaging) from the QGEO file. Because of this treatment, subgrid scale topographic features are not well represented.

Table 12 lists a detailed description of the QGEO file format. A similar table is found at the beginning of each QGEO file. Multiple cards in the same format are denoted by a line of ellipses following the card format description.

Figure 6 gives a sample of a QGEO file. A complete QGEO file is listed in the microfiche addenda.

TABLE 12. QGEO file format.

Card format	Information
(A10)	*BEGINDATA ends comment section of the QGEO file.
(A10)	*STATIONS begins station definition section of the QGEO file.
(I15)	The number of stations to be plotted on contour maps.
(20I4)	A list by station number of stations to be plotted on contour maps.
. . .	. . .
(I5)	The number of station definition cards immediately following this card.
(A4,2F10.0,I6)	The station plotting symbol, UTM easting, UTM northing, and station number.
. . .	. . .
(A10)	*RIVERS begins river (or other) map outline segment definitions.
(I5)	The number of points in this river segment. Zero points indicates the end of river segment data.
(6(F6.0,F7.0))	UTM easting-northing point coordinate pairs defining a river segment.
. . .	. . .
(A10)	*TOPO begins topographic data section of the QGEO file.
(5X,4F10.3)	Topography grid boundaries: westmost easting, southmost northing, eastmost easting, and northmost northing.
(9X,F9.3,2X,8F7.0)	Topographic data cards; each card gives UTM coordinates for the first data point on the card (UTM easting nor read), followed by eight or fewer elevations in meters. There is an increment of 1 km in UTM easting between successive data points on a card.
. . .	. . .

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD BEGIN SECTIONS HERE
BEGIN LAST LINE OF TEXT HERE
BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
PAGE NUMBER
EPA-287 (Cin.)
(4-76)

```
QGEOSTL

     THIS FILE CONTAINS  THE  AIR  MONITORING  LOCATIONS, RIVER OUTLINE
SEGMENTS, AND TOPOGRAPHY FOR THE ST. LOUIS AREA.  THE INFORMATION IS IN
THE FOLLOWING FORMAT  IN THE ORDER LISTED ( REPEATED DOTS INDICATE MORE
THAN ONE CARD IMAGE ).


      CARD FORMAT                 INFORMATION


      (A10)                       *STATIONS

      (I5)                        NUMBER OF   STATIONS  TO  BE  PLOTTED  ON
                                  CONTOUR MAPS

      (20I4)                      LIST BY STATION  NUMBER OF STATIONS TO BE
                                  PLOTTED ON CONTOUR MAPS

      ...                         ...

      (I5)                        THE NUMBER  OF STATIONS FOR WHICH TO READ
                                  DEFINING INFORMATION


     (A4, 2F10.0, I6)            STATION PLOTTING SYMBOL, UTM EASTING, UTM
                                  NORTHING, AND STATION NUMBER

     ...                          ...

     (A10)                        *RIVERS

     (I5)                         THE NUMBER   OF   POINTS  FOR  THIS  RIVER
                                  SEGMENT.  ZERO POINTS  INDICATES  THE END
                                  OF RIVER SEGMENT DATA.

     ( 6(F6.0,F7.0) )             X-Y POINT  COORDINATE  PAIRS  DEFINING  A
                                  RIVER SEGMENT

     ...                          ...

     (A10)                        *TOPO

     (5X, 4F10.3)                 TOPOGRAPHY GRID  BOUNDARIES   -  WESTMOST
                                  EASTING, SOUTHMOST   NORTHING,   EASTMOST
                                  EASTING, AND NORTHMOST NORTHING

     (9X,F9.3,2X,8F7.0)           TOPOGRAPHY DATA CARDS;  EACH  CARD  GIVES
                                  UTM COORDINATES  FOR THE FIRST DATA POINT
                                  ON THE  CARD   (UTM   EASTING  NOT  READ)
                                  FOLLOWED BY  EIGHT  OR LESS ELEVATIONS IN
                                  METRES.  THERE IS AN INCREMENT OF 1 KM IN
                                  UTM EASTING   BETWEEN   SUCCESSIVE   DATA
                                  POINTS ON A CARD.

     ....                         ...

*BEGINDATA
*STATIONS
   29 STATIONS TO BE PLOTTED ON MAP
    1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
   21  22  23  24  25  41  42  43  44
   29 STATIONS TO BE DEFINED
*101     744.18    4279.86      1
*102     742.52    4286.05      2
*103     747.59    4282.47      3
*104     747.31    4277.30      4
*105     743.71    4276.45      5
*106     738.66    4277.57      6
*107     740.18    4282.61      7
*108     748.41    4291.10      8
*109     755.80    4279.89      9
*110     747.21    4272.83     10
*111     738.81    4272.48     11
*112     733.94    4280.91     12
*113     737.74    4289.82     13
*114     744.32    4297.46     14
*115     757.11    4297.80     15
*116     762.78    4290.08     16
*117     760.56    4272.82     17
*118     743.07    4263.26     18
*119     729.76    4270.55     19
*120     723.08    4285.91     20
*121     732.41    4302.38     21
*122     741.63    4329.22     22
*123     777.32    4286.38     23
*124     749.28    4236.54     24
*125     697.45    4282.24     25
*141     742.95    4279.05     41
*142     715.71    4266.12     42
*143     760.30    4257.04     43
*144     755.86    4308.07     44
```

FIGURE 6. Example of part of a QGEO file.

```
*RIVERS    THE FOLLOWING CARDS CONTAIN RIVER OUTLINE SEGMENTS
 229
 793.8 4186.6 793.6 4187.1 792.4 4187.6 788.2 4190.4 787.3 4191.4 786.1 4193.5
 784.8 4194.7 782.6 4195.8 780.4 4196.4 777.3 4198.8 776.2 4198.5 774.4 4196.2
 773.1 4195.2 771.7 4194.8 768.2 4196.1 767.8 4196.4 766.8 4198.2 764.9 4199.2
 766.0 4198.9 766.9 4198.4 767.7 4197.1 768.4 4196.4 771.2 4195.1 772.2 4195.1
 774.1 4196.0 775.8 4198.2 776.6 4198.8 773.9 4200.7 772.8 4201.9 772.4 4202.7
 772.0 4202.8 772.0 4203.9 768.4 4206.1 766.2 4205.1 765.2 4205.1 764.6 4204.9
 763.8 4204.9 763.0 4206.2 760.2 4207.4 759.9 4208.3 759.2 4209.0 760.4 4207.9
 760.3 4208.5 759.4 4209.3 759.0 4209.0 758.9 4209.4 758.5 4209.8 756.1 4210.7
 755.4 4211.3 753.3 4212.3 752.9 4213.2 751.3 4214.9 750.1 4215.6 747.4 4216.5
 742.2 4220.5 741.2 4221.5 740.7 4222.8 739.3 4224.0 739.1 4224.9 737.3 4226.6
 738.4 4225.9 738.6 4226.3 737.6 4227.4 734.0 4229.0 731.8 4231.9 731.3 4232.8
 731.0 4234.0 730.3 4236.0 729.4 4240.3 729.2 4241.0 729.2 4242.4 729.4 4243.5
 729.4 4244.0 729.3 4244.7 729.3 4245.1 729.4 4245.7 729.7 4246.8 730.6 4248.8
 731.0 4250.8 731.8 4252.5 734.2 4254.7 736.0 4257.4 736.6 4259.1 736.7 4259.6
 736.7 4260.0 737.1 4262.0 737.2 4262.8 737.4 4263.3 737.6 4264.8 737.8 4265.9
 738.5 4267.9 739.6 4270.3 740.0 4270.7 740.8 4272.2 743.7 4275.2 744.7 4276.6
 744.7 4277.1 744.8 4277.8 745.3 4279.4 745.5 4281.1 745.5 4281.8 744.9 4283.5
 744.7 4284.5 744.5 4284.9 743.5 4286.1 742.1 4288.5 742.1 4289.5 742.3 4290.4
 742.7 4290.7 742.8 4291.2 744.5 4292.4 745.4 4294.2 745.8 4294.5 746.7 4295.9
 749.5 4298.3 749.0 4298.8 749.4 4298.6 750.0 4298.9 750.1 4299.5 749.4 4300.9
 747.8 4301.6 744.7 4300.2 744.0 4300.2 736.7 4304.8 736.0 4304.8 734.9 4305.4
 734.6 4305.8 735.6 4305.2 736.4 4305.6 734.1 4307.4 734.5 4307.5 733.8 4308.0
 733.3 4307.9 732.7 4308.0 732.0 4308.0 731.6 4307.7 730.8 4306.1 730.7 4305.6
```

```
 820.8 4285.6 821.3 4285.3 821.4 4285.7 821.9 4285.9 821.9 4287.0 822.6 4287.5
 822.9 4288.1 823.3 4287.9 824.5 4288.2 825.2 4289.6 825.6 4289.9 825.8 4290.5
 825.5 4290.9 825.0 4291.0 825.0 4291.5 824.2 4292.2 824.2 4293.2 824.1 4293.7
 823.9 4294.1 824.2 4294.6 824.6 4294.4 825.3 4295.0 825.4 4295.4 825.9 4295.3
 826.4 4295.3 827.0 4295.4 826.3 4296.6 826.7 4297.1 826.6 4297.5 826.2 4297.5
 826.2 4298.0 827.1 4298.7 827.0 4299.4 827.5 4299.5 828.5 4301.0 829.0 4301.0
 829.4 4300.7 830.0 4300.7 829.7 4300.3 830.6 4300.8 830.2 4301.1 830.7 4301.2
 831.0 4301.6 831.0 4302.1 830.4 4302.4 830.9 4302.7 830.9 4303.1 831.0 4304.1
 831.4 4303.8 831.4 4304.3 831.6 4304.7 831.5 4305.7 831.9 4305.7 832.3 4305.9
 832.3 4306.6 832.5 4307.1 832.2 4307.4 832.7 4308.0 833.1 4308.1 833.8 4308.0
 833.7 4308.5 833.7 4309.0 833.6 4309.6 834.1 4309.6 835.5 4309.0 836.4 4310.1
 836.0 4310.5 836.9 4311.0 837.5 4312.6 837.3 4313.2 837.7 4313.6 837.6 4314.1
 837.9 4315.0 837.8 4315.5 837.8 4316.8 839.2 4318.7 839.2 4319.5 839.5 4320.1
 839.1 4320.6 839.3 4321.1 839.2 4321.5 839.6 4322.6 839.6 4323.1 839.2 4323.5
 839.1 4324.2 839.1 4324.8 839.0 4325.3 839.5 4325.8 839.5 4326.2 839.1 4326.4
 839.2 4326.8 842.0 4329.3 842.4 4330.3 842.4 4330.7 843.5 4332.2 843.4 4332.7
 843.5 4333.2 843.1 4333.6 843.1 4334.1 844.1 4334.4 844.5 4334.0 845.0 4334.2
 845.1 4334.8 846.6 4336.0 846.7 4336.4 847.2 4337.2 847.6 4337.5 847.7 4338.1
 848.5 4338.7 848.8 4339.3 849.0 4340.1 849.4 4340.4 849.8 4340.4
    0 END OF RIVER OUTLINE POINTS
*TOPO     THE FOLLOWING CARDS GIVE TOPOGRAPHY DATA ON A 1 KM GRID
          654.000  4213.000    813.000  4330.000
  654.000 4213.000        270.    249.    216.    210.    215.    222.    231.    229.
  662.000 4213.000        227.    225.    236.    237.    235.    237.    236.    234.
  670.000 4213.000        237.    238.    242.    245.    244.    246.    271.    276.
  678.000 4213.000        271.    287.    305.    322.    321.    303.    293.    276.
  686.000 4213.000        277.    269.    245.    220.    220.    228.    232.    257.
  694.000 4213.000        250.    266.    254.    229.    245.    262.    265.    271.
  702.000 4213.000        267.    283.    273.    260.    253.    241.    223.    203.
  710.000 4213.000        199.    206.    217.    236.    249.    257.    254.    245.
  718.000 4213.000        238.    226.    232.    221.    229.    235.    223.    223.
  726.000 4213.000        226.    228.    226.    231.    233.    233.    231.    232.
  734.000 4213.000        232.    230.    225.    224.    225.    224.    220.    217.
  742.000 4213.000        219.    223.    227.    229.    230.    230.    230.    230.
  750.000 4213.000        230.    230.    230.    230.    230.    230.    230.    230.
  758.000 4213.000        230.    230.    230.    230.    230.    215.    130.    130.
  766.000 4213.000        151.    142.    124.    128.    142.    137.    137.    140.
  774.000 4213.000        154.    163.    157.    153.    156.    159.    154.    155.
  782.000 4213.000        154.    150.    143.    139.    138.    139.    136.    138.
  790.000 4213.000        143.    142.    140.    139.    140.    139.    139.    140.
  798.000 4213.000        141.    142.    143.    142.    142.    142.    141.    141.
```

FIGURE 6. Continued. Many similar lines are omitted in these sections.

SECTION 8

APPLICATIONS

The LIRAQ models are primarily designed to assess regional pollutant sources. The 1- to 9-km resolution used by the LIRAQ models, and the differencing schemes used (especially by LIRAQ-2S) preclude their use in assessing near source effects and render the LIRAQ models inefficient for estimating the effects of isolated point sources. Further, the two-dimensional structure of the LIRAQ models leaves them ill-suited for problems strongly dependent on the vertical resolution of emissions (e.g., effects of elevated stacks), although the LIRAQ models are well-suited for the treatment of materials with many small sources, especially if these sources are at fairly low elevations relative to the topography.

Thus, LIRAQ-1S is well-suited for the computation of CO and hydrocarbon concentrations on a regional scale, and LIRAQ-2S can reasonably treat O_3, CO, hydrocarbons, and, when they are not primarily produced by elevated point sources, the oxides of nitrogen. Although LIRAQ-2S has been modified to calculate SO_2 and $SO_4^=$, and LIRAQ-1S can calculate SO_2 concentrations, the LIRAQ models are only marginally able to represent SO_2 or sulphate because most sulfur emissions come from isolated point sources. This limitation is partly intrinsic to a two-dimensional grid model, and partly it continues because no funding has been provided to explore subgrid modeling that might alleviate the problems in treating isolated sources. Perhaps the most plausible use of LIRAQ-2S in assessing SO_x-related problems is in estimating the effect homogeneous sulfur chemistry might have on other chemical species. LIRAQ-2S results for the low-SO_2 concentrations in the San Francisco Bay Area suggest that, on a regional scale, SO_x has virtually no effect on other species included in the LIRAQ-2S reaction set. LIRAQ may also be useful in estimating the role of homogeneous photochemistry (as the model represents it) in the conversion of SO_2 to $SO_4^=$ (this is potentially large).

The treatment of SO_x in LIRAQ-2S requires two dynamic species in addition to the ten species used in treating O_3, HC, and NO_x chemistry. To a first approximation, storage and running time in LIRAQ-2S are proportional to the square of the number of species in the model. Thus, the elimination of SO_x from LIRAQ-2S would either permit a 30% increase in the number of grid elements in the model, or would reduce running costs by 30%.

Application of the LIRAQ models to the projection of future air quality or to the evaluation of proposed control strategies raises many problems that are not discussed in detail here, but which should be considered by agencies responsible for implementation or promulgation of regulations and air quality maintenance plans. Many of these problems have become evident to us as a result of the use of LIRAQ in preparing the draft Bay Area Air Quality Maintenance Plan (AQMP). A few of the more obvious problems are listed below:

1. What constitutes adequate verification for a model given that most data consist of point measurements with fallible instruments, while models generally estimate concentrations averaged over some finite domain by procedures of unknown reliability? Also, how well verified are alternative procedures such as EPA's Appendix J or the proposed EPA isopleth method?

2. For episode models (like LIRAQ), how does one relate computed pollutant concentrations to ambient air standards, especially if the meteorological data needed to drive the model are not available for worst or second worst days, and if higher pollutant concentrations are observed on differing days for different stations? (Extrapolation from the worst oxidant level in a recent year to the worst oxidant in the last decade would be more than 30% in the San Francisco Bay Area.)

3. If verification is imperfect, how does one relate computed concentrations to the standard? Is calibration allowed, or does one use results without correction? This effect can be as large as the imperfection in verification.

4. Because models are sensitive to initial and boundary conditions, how does one project initial or boundary conditions for some hypothetical future with altered emissions patterns? Bay Area experience suggests that initial and boundary conditions can have an effect of more than a factor of two on computed concentrations of O_3 in some areas.

The question of what constitutes adequate verification is clearly a regulatory decision, but one that should be affected by the requirements of the user and by a technical evaluation of the quality of model input data, available air quality data, and available alternative methodologies. The decision involves a value judgement and cannot have a clear answer on purely technical grounds.

Day-selection and model-calibration questions are technical, although they are clearly influenced by regulatory issues. The question of initial and boundary conditions is also technical, and may require a substantial increase in observations and model analyses before it can be answered. This question affects simple models like the proposed EPA isopleth method at least as severely as it affects complex models such as LIRAQ or the SAI model because these effects can be explicitly included in complex models, but must be introduced indirectly into simpler models.

The focus of the RAPS effort is on model verification and comparison. Preliminary information about the influence of O_3 and its precursors that may exist in layers aloft (Demerjian, 1977; Holets, 1977) suggests that it would be as appropriate to emphasize initial and boundary condition effects as to verify without substantial information about pollutant concentrations aloft.

SECTION 9

SENSITIVITY STUDIES

The absence of a final or reliable version of the St. Louis emissions inventory has inhibited verification studies of the St. Louis area. However, the St. Louis version of the model has been run against San Francisco Bay Area (SFBA) and St. Louis data using the preliminary version of the emissions inventory. We have been informed that the preliminary emissions inventory contained some errors. These errors lead to an underestimate of the reactive hydrocarbon emissions (Demerjian, 1977; Shreffler, 1979).

Table 13 lists the results of a study in which model sensitivity to hydrocarbon and NO_x emission variations was examined for a particular day's (July 26, 1973) SFBA climate conditions. This was a day the model produced fairly good verification results.

As Table 13 indicates, for moderate changes in hydrocarbon emissions, the model-predicted change in ozone is slightly more than linear, but model response becomes much less than linear for large hydrocarbon reductions. The reduced sensitivity for large reductions reflects the influence of the assumed background and boundary values of O_3 and hydrocarbons. There is also an inverse dependence of O_3 on NO_x emissions, which is nearly linear for moderate NO_x changes. The model also displayed strong sensitivities to upper boundary concentrations of hydrocarbons, NO_x, and, to a slightly lesser extent, O_3.

For some of the days we examined, even when hydrocarbon boundary conditions were assumed to be 10 ppb, nearly half of the total flux of hydrocarbons into the model domain between 0700 and 1000 hours came through the upper boundary condition. LIRAQ-1S was used to explore this, thus, the boundary concentrations were constant. This result is not surprising for conditions under which the model mixing depth increased from < 50 to > 1000 m over a domain of 10^4 km^2 because the

TABLE 13. LIRAQ emission sensitivity analysis results for July 26, 1973.

Reduction HC, %	0	20	40	60	80	40	80
Reduction NO, %	0	0	0	0	0	20	40
Expected worst case regionwide high-hour O_3, ppm	0.19	0.14	0.08	0.07	0.06	0.11	0.06

entrained air mass approaches 10^{10} ton. For an assumed molecular weight of 48 and a boundary concentration of 0.015 ppmV, this corresponds to more than 250 tons of hydrocarbons compared to emissions of ∿ 200 tons for the same period. One large difference in model sensitivity to emissions between the St. Louis version of LIRAQ-2S and the earlier version is that the earlier version of the model had a weaker response to emission variations (especially to NO_x emissions variations). This difference in behavior is more a reflection of our earlier use of relatively high-boundary conditions for NO and NO_2 than to any other change in model formulation.

In the course of debugging the transferred MASCON code, we found two major errors. In LIRAQ runs made using bad transport input, model sensitivity to mass inconsistency and wind speed errors were examined in a crude way. The first error was that, as a result of a difference in the way CDC FORTRAN and LLLTRAN zero arrays, when the fluxes through the upper boundary should have been upward, MASCON erroneously did not zero the downward fluxes from the previous data set. As a result, large mass inconsistencies occurred in the afternoon, although until the inversion descended, the fluxes were not seriously in error. In LIRAQ-1S, the extra mass accumulated linearly, and, because the boundary conditions were consistent and fairly low, species concentration errors were 20-100%. In LIRAQ-2S, the upper-boundary concentration is proportional to the concentration calculated just below the boundary when that concentration becomes large. As a consequence, the pollutant concentration errors in LIRAQ-2S (caused by mass inconsistency) grow exponentially. After 3 h of mass-inconsistent simulation, LIRAQ-2S calculated concentrations many thousands of times larger than it should have. This emphasizes the need for mass-consistent flux fields in the LIRAQ models.

After the mass inconsistency was corrected, a key-punching error was found that had caused the horizontal flux velocities to have the wrong units, being tenfold too large. Under these circumstances, LIRAQ rapidly swept the initial concentrations out of the grid and approached a state in which the mean layer concentrations were nearly constant and determined by the boundary conditions (and a few plumes from large emission sources). In contrast, the surface concentrations reflected the surface-to-mean-layer ratio calculated as a function of mixing depth, emissions rate, deposition velocity, and K_z. Ozone was generated at low concentrations but with a fairly reasonable temporal variation. These runs demonstrate the asymptotic behavior expected of LIRAQ.

We also compare concentrations computed using LIRAQ-2S (Figures 7 and 9) to those calculated using LIRAQ-1S (Figures 8 and 10) for a simulation in which point sources are the dominant sources. Figures 7 and 8 are in reasonably close agreement, demonstrating that the differencing scheme used in LIRAQ-2S introduces fairly minor errors in even these plume calculations. However, Figures 9 and 10 display large differences in concentration near the lower righthand corner. This is an artifact of the LIRAQ-2S boundary condition and its interaction with a strong source at the model domain boundary. Because the boundary flow involves the concentration just inside the boundary, a strong source on an upwind boundary has the effect of creating a virtual source of comparable magnitude just outside the model domain. As a result, LIRAQ-2S overestimates the flux entering at the lower righthand corner and LIRAQ-2S overestimates SO_2 at all points influenced by air from that region.

Finally, we provide Figures 11 and 12 showing sample ozone concentrations computed for a particular simulation of day 195, 1976. Because no final version of the

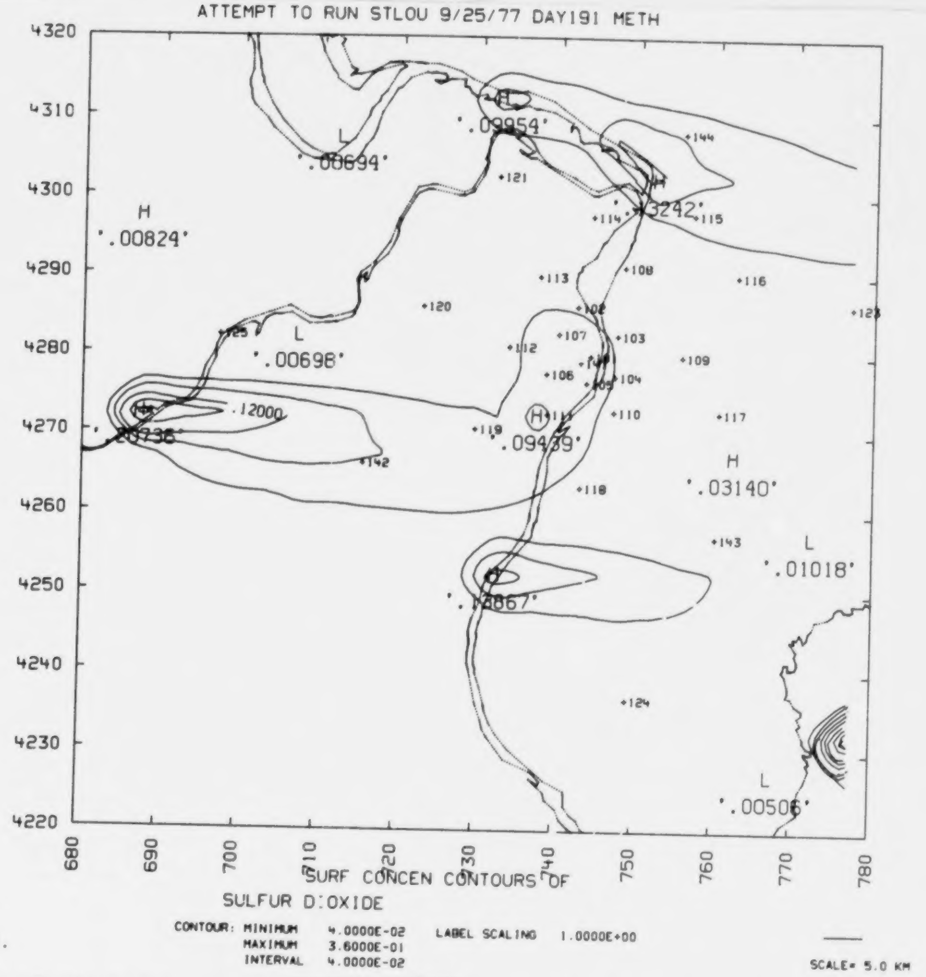
ATTEMPT TO RUN STLOU 9/25/77 DAY191 METH
4320
4310
4300
4290
4280
4270
4260
4250
4240
4230
4220
680
690
700
710
720
730
740
750
760
770
780
H
'.00824'
L
'.00694'
'.09954'
'.3242'
'.00698'
.12000
'.20736'
'.09439'
H
'.03140'
L
'.01018'
'.12867'
L
'.00506'
SURF CONCEN CONTOURS OF
SULFUR DIOXIDE
TIME
10: 0.
JULY 191
CONTOUR: MINIMUM 4.0000E-02
MAXIMUM 3.6000E-01
INTERVAL 4.0000E-02
LABEL SCALING 1.0000E+00
SCALE= 5.0 KM

FIGURE 7. Surface concentration map for SO_2 as calculated by LIRAQ-2 for 1000, day 191, 1975.

emissions inventory has been available to us, the calculated fields (which are not in good agreement with observation), must be viewed as provisional also. If the final emissions inventory yields more reactive hydrocarbons emissions, as has been suggested, then the agreement between model and observation would be improved. The differences between Figures 11 and 12 reflect the difference between surface and mean layer concentrations. The computed ozone concentration fields show a general increase as one moves away from the upwind (southern) boundary. The other noticeable features are strong minima at and downwind from major point sources of NO_x and a weak maximum over the city.

BEGIN FIRST LINE OF TEXT HERE
TYPING GUIDE SHEET
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD HERE BUTTONS LINE

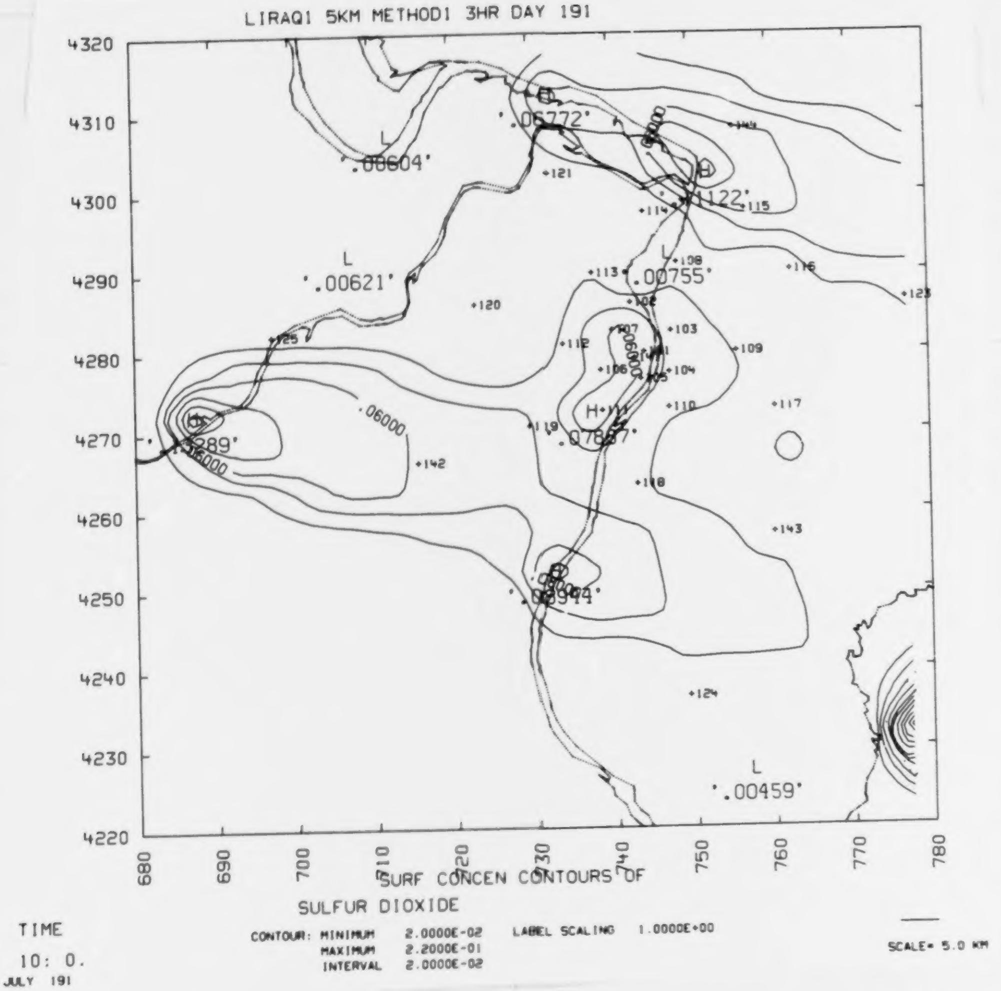
LIRAQ1 5KM METHOD1 3HR DAY 191
4320
4310
4300
4290
4280
4270
4260
4250
4240
4230
4220
680
690
700
710
720
730
740
750
760
770
780
L
'.00604'
'.06772'
'.1122'
L
'.00621'
L
'.00755'
'.06000
'.1289'
.06000
H
'.07887'
'.08944'
L
'.00459'
+121
+114
+115
+116
+113
+108
+123
+120
+102
+107
+103
+125
+112
+104
+106
+109
+105
+110
+117
+119
+142
+118
+143
+124
SURF CONCEN CONTOURS OF
SULFUR DIOXIDE
TIME
10: 0.
JULY 191
CONTOUR: MINIMUM 2.0000E-02
MAXIMUM 2.2000E-01
INTERVAL 2.0000E-02
LABEL SCALING 1.0000E+00
SCALE= 5.0 KM

FIGURE 8. Surface concentration map for SO_2 as calculated by LIRAQ-1 for 1000, day 191, 1975.

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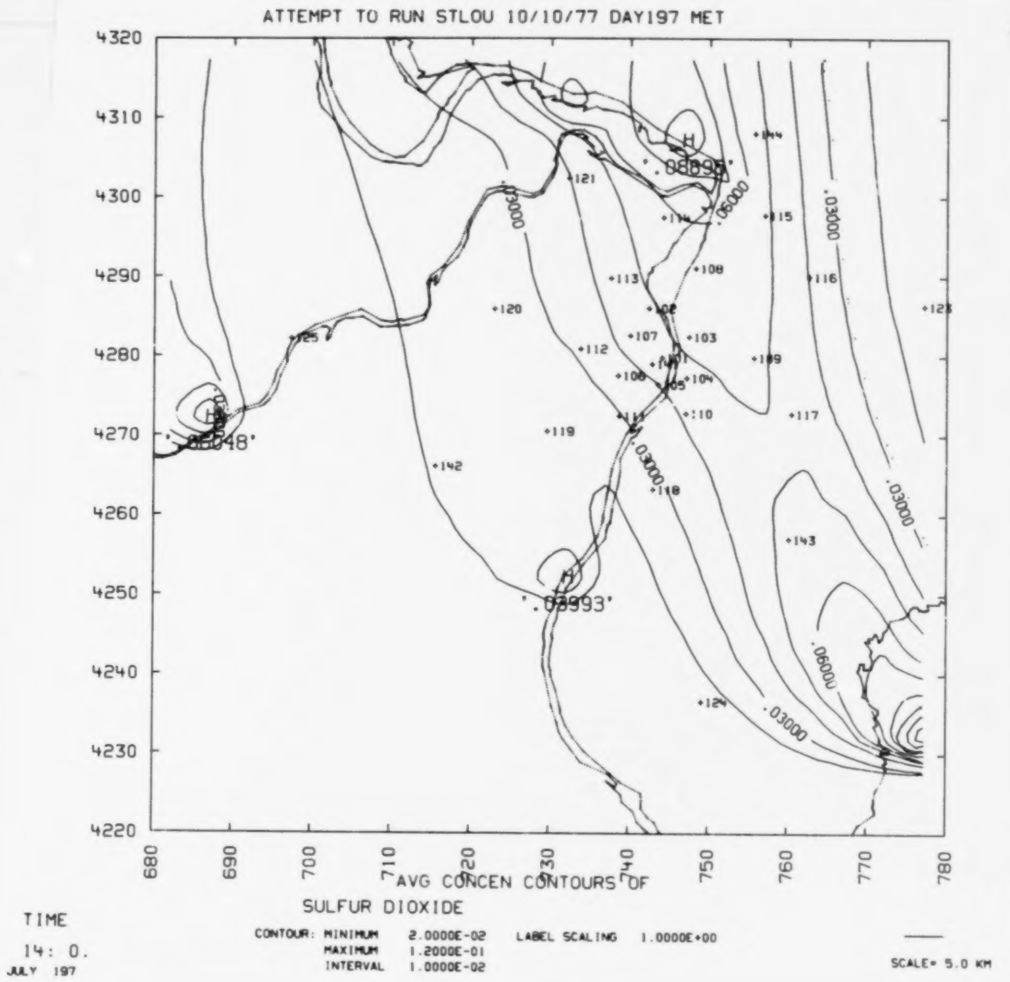
ATTEMPT TO RUN STLOU 10/10/77 DAY197 MET
4320
4310
4300
4290
4280
4270
4260
4250
4240
4230
4220
680
690
700
710
720
730
740
750
760
770
780
AVG CONCEN CONTOURS OF
SULFUR DIOXIDE
TIME
14: 0.
JULY 197
CONTOUR: MINIMUM 2.0000E-02
MAXIMUM 1.2000E-01
INTERVAL 1.0000E-02
LABEL SCALING 1.0000E+00
SCALE= 5.0 KM
H
'.08898'
'.08048'
'.08993'
.03000
.06000
+144
+121
+114
+115
+113
+108
+116
+120
+102
+107
+103
+125
+112
+109
+106
+101
+104
+105
+111
+110
+117
+119
+142
+118
+143
+124

FIGURE 9. Mean layer concentration map for SO_2 as calculated by LIRAQ-2 for 1400 day 197, 1975. The eastern boundary was poorly chosen in this example. A large SO_2 source is located just inside the upwind boundary and is artificially augmented by the LIRAQ-2 boundary condition.

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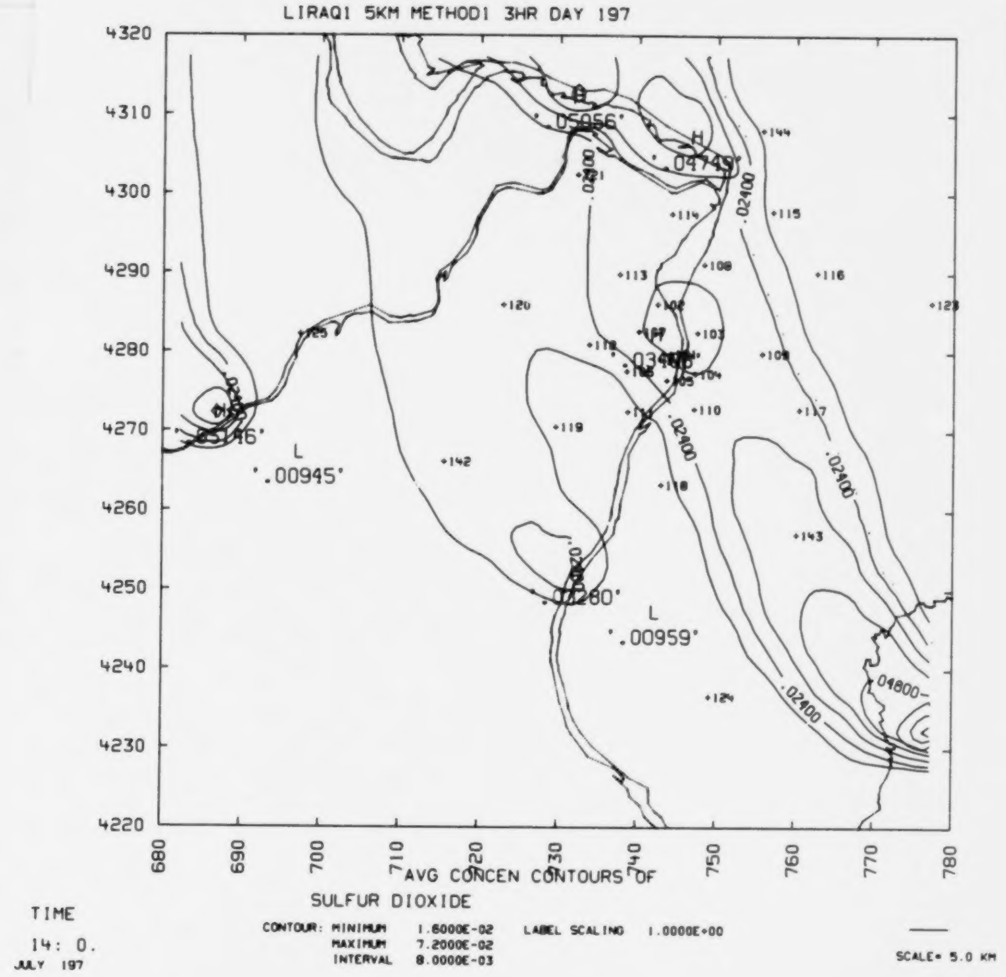
LIRAQ1 5KM METHOD1 3HR DAY 197
4320
4310
4300
4290
4280
4270
4260
4250
4240
4230
4220
680
690
700
710
720
730
740
750
760
770
780
H
'.05056'
H
'.04749'
.02400
.02400
'.03446'
'.03146'
L
'.00945'
.02400
.02400
'.02280'
L
'.00959'
.02400
.04800
+144
+115
+116
+114
+113
+108
+120
+123
+125
+103
+109
+119
+110
+117
+142
+118
+143
+124
AVG CONCEN CONTOURS OF
SULFUR DIOXIDE
TIME
14: 0.
JULY 197
CONTOUR: MINIMUM 1.6000E-02
MAXIMUM 7.2000E-02
INTERVAL 8.0000E-03
LABEL SCALING 1.0000E+00
SCALE= 5.0 KM

FIGURE 10. Mean layer map for SO_2 as calculated by LIRAQ-1 for 1400, day 197, 1975. The LIRAQ-1 boundary flux is unaffected by the location of a strong source just inside the upwind boundary.

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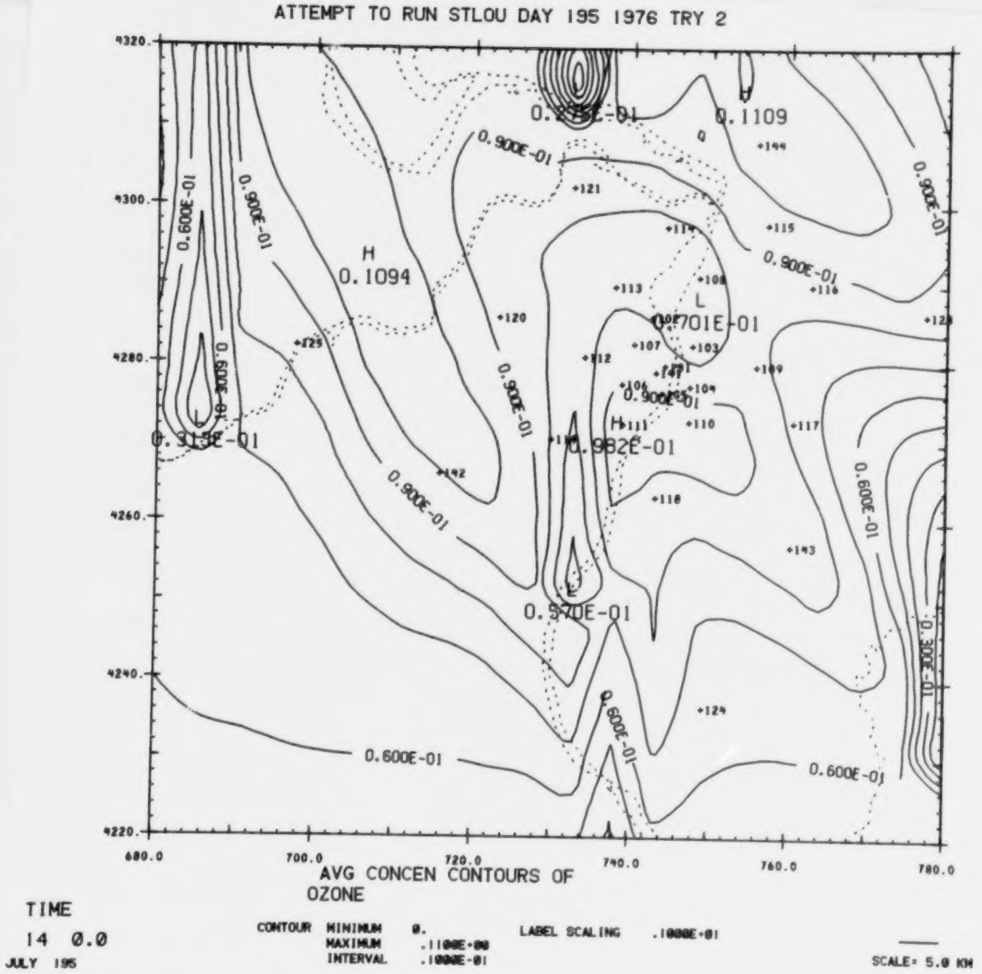

FIGURE 11. Computed mean layer ozone concentrations for day 195, 1976 at 1400.

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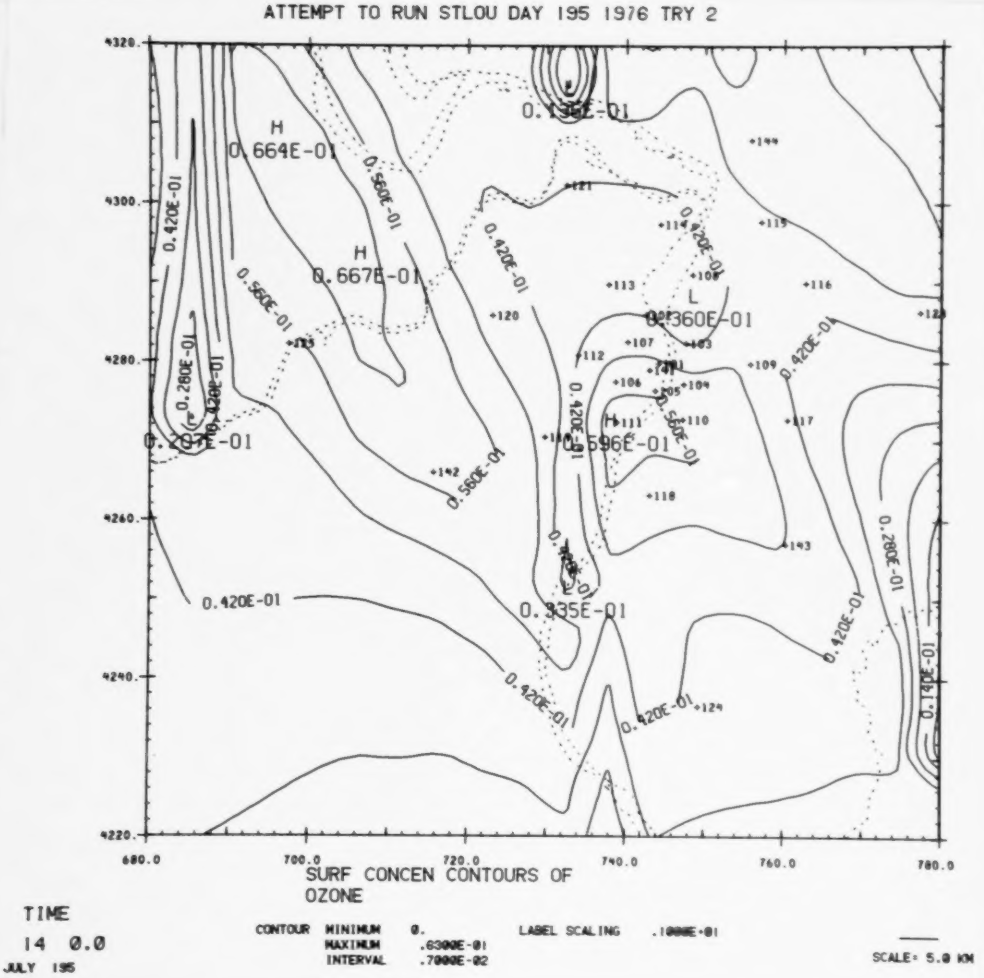

FIGURE 12. Computed surface ozone concentrations for day 197, 1976 at 1400.

SECTION 10

CONCLUSIONS AND CONTROVERSIES

Under an interagency agreement with the EPA, LLL has modified the LIRAQ models for participation in the Regional Air Pollution Study (RAPS). The modifications to the LIRAQ models have included:

1. Modifications to the chemical mechanism in LIRAQ-2S, so that the model now includes a representation of the homogeneous gas phase photochemistry for conversion of SO_2 to $SO_4^=$, and an update of the reaction rates and mechanisms to reflect the data available in March 1976.

2. Several input checks (in both models) to ensure that all input files — source, meteorology, and initial condition files refer to the same day.

3. Changes in the topographic input designed to improve the versatility of river and coastline-plotting routines.

In addition, we have:

1. Developed processors that generate LIRAQ input files from RAPS data tapes.

2. Converted MASCON and VERF processors to standard FORTRAN and exported them to Lawrence Berkeley Laboratory (LBL).

3. Provided documentation.

However, several unresolved questions remain. Because we have not yet been provided with an emissions inventory considered reliable by the EPA, little can be said about how reliable or suitable our estimates are for initial conditions, boundary conditions, or mixing depths. Further, there are indications of errors in the RAPS pollutant measurements. Recorded O_3 measurements at three RAPS stations are known to be about two-fold high, and RAPS stations frequently report CO measurements of roughly 50 ppb; the background Northern Hemisphere CO-mixing ratio is thought to be between 100 and 200 ppb. Although the RAPS seems likely to be the best existing air quality data base, inconsistencies and errors in it undermine our confidence in its use. Thus, data errors continue to contribute to verification discrepancies, as does the problem of comparing computed spatially averaged concentrations with measured point concentrations.

Sensitivity experiments for St. Louis and San Francisco Bay Area conditions indicate that model predictions for O_3 are sensitive to the upper boundary condition, a sensitivity common to at least some other models (Demerjian, 1977). There are almost no data in the standard RAPS data base that can be used to guide the choice of upper boundary conditions, although pertinent data were taken in some of the special studies sponsored by RAPS. Unless data from the special studies are used, pollutant concentrations aloft will provide a set of poorly known parameters capable of strongly influencing model predictions. The treatment of such factors will be a central issue in questions of verification and in future applications of complex models such as control-strategy evaluation.

At present, there is no adequate basis for judging LIRAQ performance. The interim St. Louis source inventory is thought to be questionable, and our recent Bay Area studies (work now in progress) have demonstrated that several Bay Area days can be simulated reasonably well by LIRAQ, but only if adjustments are made in upper boundary concentrations. As long as boundary conditions are poorly known, verification performance will remain difficult to judge.

Of the changes made in LIRAQ for RAPS, the update of the chemical mechanism and changes in the treatment of the steady-state species for LIRAQ-2S, the consistency checks added to the input, and the transfer of VERF and MASCON codes to LBL, all are likely to be immediately used by other LIRAQ users. Most of these features have been used by the BAAQMD in support of the San Francisco Bay Area Air Quality Maintenance Plan. The addition of $SO_2/SO_4^=$ chemistry seems less likely to be useful.

Recommended future changes in LIRAQ include a further updating of model chemistry,* removal of SO_2, $SO_4^=$, and HNO_3 from LIRAQ-2S, and the addition of peroxyacylnitrates, a simplification of LIRAQ-2S numerics, and (possibly) an expansion of the LIRAQ-2S grid. These changes should result in either a material decrease in running time or an increase in spatial resolution.

The LIRAQ model makes the assumption that the dispersion, transport, and transformation of pollutants can be represented by treating only a single atmospheric layer extending from the surface to the normal temperature inversion. This assumption, coupled with the assumed behavior of pollutant concentration in the vertical, will be most valid when:

1. Pollutants are emitted primarily at the surface or below the inversion (the single-layer model does not keep track of pollutants emitted above the inversion).
2. Vertical dispersion is limited by a strong and persistent inversion.
3. Vertical mixing in the layer is rapid compared with horizontal transport across a grid cell.
4. Pollutant concentrations in the layer result primarily from emissions within the layer rather than prescribed fluxes through the inversion.

In the San Francisco Bay Area, most of these conditions are met most of the time when:

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*This is presently being carried out under funding from the BAAQMD.

1. A large fraction of the important pollutants are emitted from automobiles and other surface sources.
2. An inversion is nearly always present.
3. The atmosphere is stable (if stable, the inversion tends to be shallow so that vertical mixing need not extend a great distance; conversely, if the inversion is high, mixing is rapid).

Application of the LIRAQ model to St. Louis, rather than the typical west-coast-maritime, inland-valley regime for which it was designed, strains the condition of the single-layer assumption. Many emission sources, particularly for SO_2, are elevated point sources that persist in the inversion and then may be mixed to the surface as the inversion rises, a process LIRAQ does not treat. The atmospheric structure in St. Louis often involves multiple, weak or nonexisting inversions creating layers that are alternately coupled and isolated during a diurnal cycle, a process crudely treated in LIRAQ. Vertical mixing can be rapid during daylight hours, but is often weak, thus the height of mixing (or single-layer depth) is not always well-defined. The elevated emissions and the multiple stable layers coupled with the diurnal cycle mean that pollutant concentrations in the single layer may often be strongly influenced by pollutants not emitted in that layer. Taken together, the characteristics of LIRAQ and St. Louis indicate that expectations of good verification should not be high and verification and analysis should be carefully pursued.

The preliminary results of LIRAQ simulations of O_3 in St. Louis involve substantial underprediction. This could reflect basic model error, improper boundary/initial conditions, emissions inventory errors or excessive mixing of NO_x from elevated sources down to the surface.

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REFERENCES

Bass, A., A. Q. Eschenroeder, B. A. Egan. 1977. The Livermore Regional Air Quality Model (LIRAQ) A Technical Review and Market Analysis. Environmental Research and Technology, Inc., Document P-2348-1, report to the NSF.

Bates, D. R. and P. B. Hays. 1967. Atmospheric Nitrous Oxide. Planet. and Space Sci. 15:189.

Boris, J. and D. L. Book. 1973. Flux-Corrected Transport: I. SHASTA, a Fluid Transport Algorithm That Works. J. Comput. Phys. 11:38.

Demerjian, J. 1977. EPA, Research Triangle Park, N.C., private communication.

Dickerson, M. H. 1973. A Mass Consistent Wind Field Model for the San Francisco Bay Area. Lawrence Livermore Laboratory Report UCRL-74265.

Dickerson, M. H. 1978. MASCON — A Mass Consistent Atmospheric Flux Model for Regions with Complex Terrain. J. Appl. Meteor. 17:241-253.

Duewer, W. H., M. C. MacCracken, and J. J. Walton. 1978. The Livermore Regional Air Quality Model: II. Verification and Sample Application in the San Francisco Bay Area. J. Appl. Meteor. 17:274-311.

Hampson, R. F. and D. Garvin. 1975. Chemical Kinetics and Photochemical Data for Modeling Atmospheric Chemistry. National Bureau of Standards, Washington, D.C., NBS Technical Note 866.

Hecht, T. A., M. K. Liu, and D. C. Whitney. 1974. Mathematical Simulation of Smog Chamber Photochemical Experiments. Environmental Protection Agency, Research Triangle Park, NC, Final Report Contract 68-02-0580.

Hecht, T. A., J. Seinfeld, and M. Dodge. 1974. Further Development of a Generalized Kinetic Mechanism for Photochemical Smog. Environ., Sci. & Tech. 8:327.

Holets, S. G. 1977. Bay Area Air Pollution Control District, San Francisco, CA, private communication.

Johnston, H. S. and G. S. Selwyn. 1975. New Cross Sections for the Absorption of Near-Ultraviolet Radiation by N_2O. Geophys. Res. Letters. 2:549-551.

MacCracken, M. C. 1975. User's Guide to the LIRAQ Model: An Air Pollution Model for the San Francisco Bay Area. Lawrence Livermore Laboratory Report UCRL-51983.

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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

MacCracken, M. C. and G. D. Sauter (eds.). 1975a. Development of an Air Pollution Model for the San Francisco Bay Area. Final Report, Lawrence Livermore Laboratory Report UCRL-51920, Vol. 1.

MacCracken, M. C. and G. D. Sauter (eds.). 1975b. Development of an Air Pollution Model for the San Francisco Bay Area. Final Report, Lawrence Livermore Laboratory Report UCRL-51920, Vol. 2, Appendices.

MacCracken, M. C., D. J. Wuebbles, J. J. Walton, W. H. Duewer and K. E. Grant. 1978. The Livermore Regional Air Quality Model: I. Concept and Development. J. Appl. Meteor. 17:254-272.

Noxon, J. F. 1975. Nitrogen Dioxide in the Stratosphere and Troposphere Measured by Ground Based Absorption Spectroscopy. Science. 189:547.

Rasmussen, K. H., M. Takeri, and R. L. Kabil. 1975. Global Emissions and Natural Pollutants. Water Air and Soil Pollu. 4:33.

Rasmussen, R. A. 1977. Oregon Graduate Center, Eugene, Oregon, private communication.

Reid, L. E. and S. D. Reynolds. 1979. A Comparison of the Technical Features of the SAI Airshed Model and the Livermore Regional Air Quality (LIRAQ) Model. Report EF79-33R, Systems Applications, Incorporated, San Rafael, CA.

Sauter, G. D. 1978. A Workshop on the Livermore Regional Air Quality (LIRAQ) Model. Lawrence Livermore Laboratory, private communication.

Shreffler, J. 1977. EPA, Research Triangle Park, N.C., private communication.

Seiler, J. 1974. Cycle of Atmospheric CO. Tellus. 26:116.

Stullich, T. W., M. C. MacCracken, and K. E. Grant. 1978. User's Guide to the MASCON Model: A Mass Consistent Atmospheric Flux Sub-Model to LIRAQ. Lawrence Livermore Laboratory Report UCRL-52400.

Systems Applications, Inc. 1977. A Discussion of the Livermore Regional Air Quality Model and the SAI Urban Airshed Model. Prepared by Systems Applications, Inc., San Rafael, CA, Report ES.

Trijonis, J. C. and K. W. Arledge. 1975. Utility of Reactivity Criteria in Organic Emission Control Strategies for Los Angeles. TRU Report, Contract No. 68-02-1735 for EPA.

Whitten, G. Z. and H. Hogo. 1977. Mathematical Modeling of Simulated Photochemical Smog. EPA Report 600/3-77-0111, U. S. Environmental Protection Agency, Office of Research and Development, Research Triangle Park, N.C.

APPENDIX A

LIST OF PROCESSORS AND ASSOCIATED FILES

This appendix consists of a list of all the processors used with the LIRAQ models, and the files needed to compile and execute the various processors. Table A-1 lists the various independent processors available with the LIRAQ models in treating RAPS/RAMS data and Tables A-2 to A-9 list the various files associated with each processor. Appendices B to I describe the processors, Appendix J describes the control card decks and Appendix K provides guidelines for estimating run times.

TABLE A-1. Independent processors associated with LIRAQ models.

Routine	Purpose	Location of control cards
Source Processor	Converts RAPS emissions to LIRAQ QSORxx files	Data cell library SORPROC file SPRCLGO
UADATA	Graphical display of RAMS data	Data cell library MASCON file UADCLGO
Q-Processor	Generates QICON, edits RAMS data generates MPROC input	Data cell library MASCON file QPRCLGO
M-Processor	Averages RAMS data to agree with MASCON data intervals	Data cell library MASCON File MPRCLGO
MASCON	Generates mass-consistent flux fields (QTRANx) from averaged RAMS data	Data cell library MASCON file MSCNLGO
LIRAQ-1S	Computed concentrations of nonreactive species	Data cell library LIRAQ file LR1SLGO
LIRAQ-2S	Computed concentrations of reactive species	Data cell library LIRAQ file LR2SLGO
VERF	Compares computed and measured concentrations	Data cell library LIRVERF file VERFLGO

TABLE A-2. Files associated with the source processor.

Associated files	Type	Function
QPPRCLGO*+	Control card	Load and execute the source processor, acquire needed input files, dispose of output.
AREABN+	Binary input	Area sources for selected day.
PTBN+	Binary input data	Point sources for selected day.
RDARBN	Binary input data	For loader.
RDARSYM	Symbol table	For loader.
RDPTBN	Binary	For loader.
RDPTSYM	Symbol table	For loader.
AREA+	Card image-output	Card image version of AREABN.
POINT+	Card image-output	Card image version of PTBN.
INPUTS*+	Instructions-input	Run parameters.
GRIDES	Input data	RAPS grid data.
SPRCBN	Binary	For loader.
SPRCSYM	Symbol table	For loader.
QSOR00-QSOR24+	Output	LIRAQ compatible emissions data to be archived for future use.
OUTPUT	Diagnostic output	Error messages, summary of emissions.

COMMENTS: The source processor was developed by H. Walker of LLL. It is described in Appendix B.

*Must be altered by user.

+Will normally vary from run to run.

TABLE A-3. Files associated with UADATA.

Associated Files	Type	Function
UADCLGO/INPUT[*][+]	Control cards	Update, compile, and execute METGRAF, fetch needed files, dispose of output.
UADDK	Input	Contains update commands, river data for map.
RAMS[+]	Data input	Meteorological and pollutant data = RAMS HISTORY file.
RAPSGRD	Data input	RAPS grid information.
GPAC	Systemic	LBL graphics library file.
ULIB	Systemic	LBL graphics library file.
SYMTAB	Systemic	Symbol table used in compiling.
GRUMP	Systemic	LBL systems library file.
OUTPUT[+]	Output	Echoes inputs, graphical display of RAMS data.

COMMENTS: UADCLGO Must be modified to select appropriate input files RAMSDAT and UADDK for every run. UADDK must be modified if update instructions are to be used (i.e., if UADATA is to be changed). RAMS should be taken from the appropriate archival tape. It is the same as RAMSDAT used by the Q-Processor. A sample UADCLGO is stored on data cell and can be accessed by "FETCHPS, MASCON, UADCLGO, UADCLGO . . .". This code was generated by W. Johnston of LBL. UADATA is not essential to the operation of the LIRAQ codes, but is a tool to be used in appraising RAMS data. UADATA is documented in Appendix E and in the MASCON User's Guide (Stullich et al., 1979).

[*] Must be modified by user.

[+] Will normally vary from run to run.

TABLE A-4. Files associated with Q-Processor.

Associated Files	Type	Function
QPRCLGO*+	Control card	Load and execute the Q-Processor, acquire needed input files, dispose of output.
MIXHGT+	Data	Mixing depths.
RAMSDAT+	Data	RAMS data for a selected day.
QPINPUT*+	Data/instructions	Gives latitude, (°) local noon(s) and editing instructions, if any.
PASLIB	Systemic	For loader
QPRCBN	Binary	For loader
QPMCOM	Input	Preface to QPMET (inserts comment cards in QPMET).
QICON+	Output	To be archived for future use by LIRAQ-1, LIRAQ-2, and VERF.
QPMET+	Output	To be archived for future use by M-Processor.
OUTPUT+	Diagnostic	Echoes input, provides some error diagnostics.

COMMENTS: Programmed by H. Walker of LLL. It is described in Appendix C. When the Q-Processor is executed, QPRCLGO must be modified to select the correct QPINPUT and RAMSDAT files for the data set in question. Titling information for fiche output must be modified and an appropriate designator for the archival addresses of QICON and QPMET must be specified. See Appendix C and the MASCON User's Guide (Stullich et al., 1979).

*Must be modified by user.

+Will normally vary from run to run.

TABLE A-5. Files associated with M-Processor.

Associated files	Type	Function
MPRCLGO*+	Control cards	Loads and executes M-Processor, acquires and disposes of files, has attached input that gives start time and date, number of hours between output data sets.
QPMET+	Input	Provides reformated meteorological data, output from Q-Processor.
MPCRBN	Binary	For loader
QMET+	Output	To be archived for future use by MASCON.
OUTPUT+	Diagnostic	

COMMENTS: MPRCLGO must be modified to select appropriate QPMET file from archive, select an appropriate archival address for QMET, and generate appropriate titling. The M-Processor was developed by K. E. Grant of LLL. It is described in Appendix D and in the MASCON User's Guide (Stullich et al., 1978).

*Must be modified by user.

+Will normally vary from run to run.

TABLE A-6. Files associated with MASCON.

Associated files	Type	Function
MSCNLGO[*][+]	Control card	Load and execute MASCON, acquire and dispose of files. Set computing limits for job.
QMRUN[*][+]	Input	Sets run parameters (physical and temporal domains, grid interval, etc.).
QGEO	Data/input	Gives map information.
QMET[+]	Data/input	Gives meteorological information. Generated by M-Processor.
MSCNBN	Binary	For loader
SCLGOF	Systemic	LBL Graphics Library file
ULIB	Systemic	LBL Graphics Library file
TV80TLB	Systemic	LBL Graphics Library file
SYNTAB	Symbol table	For loader
QHSP[+]	Output	Diagnostic
QFLXCK[+]	Output	Diagnostic
QDIAG[+]	Output	Diagnostic
QGRAPH[+]	Graphics	Diagnostic
QTRANx[+]	Output	A family of files to be archived for future use by LIRAQ-1 or LIRAQ-2.

COMMENTS: MASCON is documented in the MASCON User's Guide (Stullich et al., 1978). In order to execute MASCON, MPRCLGO must be edited to select appropriate QMRUN, QGEO, and QMET files, generate appropriate titles and archival addresses for the QTRANx files. QGEO does not change unless a different city (e.g., St. Louis or San Fransicso) is selected. QMET files are specific to an urban area, date, and meteorological data interval. QMRUN files must be modified for every model run, their content is described in Appendix F and in Stullich et al. (1978).

[*] Must be modified by user.

[+] Will normally vary from run to run.

TABLE A-7. Files associated with LIRAQ-1S.

Associated files	Type	Function
LR1SLGO*+	Control card	Loads and executes LIRAQ-1S, sets time limits, acquires input files and disposes of output.
QSRUN*+	Input	Sets run domain (spatial and temporal), grid size, selects output, gets boundary conditions, etc.
QGEO	Data	Map data.
QICON+	Data	Pollutant concentration data.
QTRAN0-QTRANx+	Data	Transport coefficients, K_z, mixing depths and transmissivities. Produced by MASCON.
QSOR00-QSOR24+	Data	Emissions data. Produced by source processor.
LRISBN	Binary	For loader.
SCBN	Systemic	LBL Graphics Library file.
ULIB	Systemic	LBL Graphics Library file.
TV80TLB	Systemic	LBL Graphics Library file.
LRISSYM	Symbol table	For loader.
QHSP+	Output	Tabular output. Diagnostic, used by some applications oriented post processors, used to evaluate.
QSREC+	Output	Archival, used by VERF.
QTYM+	Output	To fiche.
QGRAPH+	Output	To fiche.

COMMENTS: LIRAQ-1S was developed by K. E. Grant and M. C. MacCracken of LLL. W. and N. Johnston of LBL participated in its conversion to LBL. It has been documented in a formal users guide (MacCracken, 1975). The present version has been modified to accept more general map data, and check dates on various input files. In order to execute LIRAQ-1S, LRISLGO and QSRUN must be modified and appropriate QGEO, QICON, QTRANx, and QSORxx files must be acquired from archive. See Appendix G for a description.

*File must be modified by user.

+File will normally differ from run to run.

TABLE A-8. Files associated with LIRAQ-2S.

Associated files	Type	Function
LR2SLGO[*,+]	Control card	Loads and executes LIRAQ-2S. Sets computing limits, acquires and disposes of files.
QSRUN[*,+]	Input	Sets run parameters (spatial and temporal domains, etc.).
QRAD	Data	Photodissociation rates as a function of zenith angle.
QGEO	Data	Map information.
QTRAN0-QTRANx[+]	Data	Transport data, transmissivity data.
QSOR00-QSORxx[+]	Data	Emissions data.
QICON[+]	Data	Initial conditions.
LR2SPL	Binary	For loader.
SCBN	Systemic	LBL Graphics Library file.
ULIB	Systemic	LBL Graphics Library file.
TV80TLB	Systemic	LBL Graphics Library file.
LR2SSYM	Symbol table	For loader.
QHSP[+]	Output	Primarily diagnostic, but used by some applications oriented post processors.
QSREC[+]	Output	Archival, used by VERF.
QREST[+]	Output/input	Archival, used to restart a problem.
QGRAPH[+]	Graphics	Diagnostic output graphics.
QSTEP[+]	Diagnostics	Run diagnostic output.

COMMENTS: LIRAQ-2S developed by J. J. Walton, W. H. Duewer, D. J. Wuebbles, M. C. MacCracken and K. E. Grant of LLL. Much of the work involved in converting LIRAQ-2S to LBL was done by W. and N. Johnston of LBL. Some work was done by M. G. Paley and W. Day, consultants to the BAAPCD. The coding of the original version of the model has been described in a formal users guide (MacCracken, 1975). See Appendix H for a description.

[*] File must be modified by user for each run.

[+] File will normally vary from run to run.

TABLE A-9. Files associated with VERF.

Associated files	Type	Function
VERFLGO[*][+]	Control card with attached input	Load and execute VERF. Assemble and dispose of files. Selects pollutants, time domain.
QSREC[+]	Data	Model computed concentrations.
QICON[+]	Data	Station observations.
VERFBN	Binary	For loader.
SCLGOF	Systemic	LBL Graphics Library file.
ULIB	Systemic	LBL Graphics Library file.
OUTPUT[+]	Diagnostic	Gives error messages.
GRAPHICS[+]	Output	Compares model with observation.

COMMENTS: VERFLGO must be modified for every run to ensure that the appropriate QSREC and QICON files are selected. In addition, appropriate time domains must be specified in the attached input. See Appendix I for a description.

[*] File must be modified by user.

[+] File will normally vary from run to run.

APPENDIX B

NEDS/RAPS SOURCE PROCESSOR

The source processor (SORP) reads pollutant source data from St. Louis and produces a set of hourly QSOR files for input to LIRAQ.

PROCESSOR DESCRIPTION

The source processor has been coded in FORTRAN to be compiled with the CDC FTN 4.4 compiler.

First, the source processor defines the LIRAQ grid, a regular rectangular north-east grid with grid cells that may be chosen from 1 to 5 km on a side. The size of the grid cells is read from the file INPUTS along with other grid parameters that may be input. If other parameters are not specified, SORP chooses the largest grid within UTM east coordinates 654 and 813 and UTM north coordinates 4213 and 4330. The grid points are integer multiples of the grid size. If the user specifies the LIRAQ grid and requires more than 159 grid cells along the east axis or 117 grid cells along the north axis, the code will have to be recompiled with larger dimensions for the two-dimensional arrays. If the UTM east coordinate of the grid is specified by the user, the remaining grid parameters must also be specified. The processor can also be run with grid cells larger than 5 km. However, if this is done, the user must supply a full description of the grid domain to be considered (i.e., the interval and the UTM coordinates of the grid boundaries must be directly specified. No defaults are available.).

The main data structures in the source processor are a set of two-dimensional arrays. These arrays are dimensioned so that each array element corresponds to a LIRAQ grid cell. The first index of the array specifies grid position along the north axis. The second index specified grid position along the east axis. The array element (1,1) corresponds to the cell in the southwest corner of the grid. An entry in one of these arrays is the emission rate in g/s of a particular pollutant class within the corresponding LIRAQ grid cell. Thus, there is one two-dimensional array for each pollutant of the following classes:

Elevated SO_x
Elevated particulate
Elevated NO_x
Elevated CO
Elevated HC1
Elevated HC2
Elevated HC4
Surface particulate

Surface NO_x
Surface CO
Surface HC1
Surface HC2
Surface HC4

The input data are processed one hour at a time. Point sources from input file POINT are processed first with one card examined at a time. From the UTM coordinates on the card, the LIRAQ grid cell that contains the source is determined. The emission rates are added to the corresponding elements of the elevated or surface pollutant arrays, depending on the height field; elevated sources are 20 m or more above the ground. All input emission rates are converted from kg/h to g/s for internal use by LIRAQ. After all the point sources for an hour have been completed, the area sources are read from input file AREA along with RAPS grid information from GRIDES and processed one RAPS grid cell at a time. Using the area of the grid cell, the emission rate per km^2 in g/s for each pollutant is computed. For each km^2 of the RAPS grid cell, we determine the LIRAQ grid cell in which it resides. For each pollutant, the emission rate per km^2 is added to the appropriate array element. All area sources are assumed to be surface sources. After all the input has been processed, the data are written in the required format to the QSOR file for the hour. For both POINT and AREA input data the RAPS hydrocarbon species (non-reactive, paraffin, olefin, aromatic, aldehyde) are converted to the LIRAQ hydrocarbon classes according to the following formulae:

$$\text{HC1} = 44 * (1.2 * \text{olefin} + 0.5 * \text{aromatic})$$

$$\text{HC2} = 58 * (1.3 * \text{paraffin} + 0.5 * \text{aromatic} + 0.1 * \text{non-reactive})$$

$$\text{HC4} = 38 * (1.2 * \text{aldehyde})$$

Since the input data for speciated hydrocarbons are measured in moles per hour, these equations contain the conversion constants (molecular weights of the LIRAQ prototype species) required to change the RAPS data to grams per hour on the basis of the estimated average molecular weight of the LIRAQ hydrocarbon classes as well as reactivity factors designed to convert RAPS prototype species into LIRAQ classes. After completion of the output, the hourly emissions integrated over the grid are written into DAYFILE so that the user can check for gross errors. After all hours have been used, the data for hour 23 is written again to QSOR24, creating a copy of QSOR23. Figure B-1 is a flowchart for this process.

INPUT FILES

Pollutant source data are contained in three files. The file POINT contains all point source data. GRIDES describes all of the RAPS grid cells and is used with input file AREA which contains all the area source emission rates. These are all BCD files. The date available on tape from EPA/RAPS is all in binary form, consequently three short conversion programs have been written to perform the required transformation to BCD format.

POINT

Point source data are read in binary form from the EPA/RAPS tape. The format of the binary data is described in a communication from EPA/RAPS as follows:

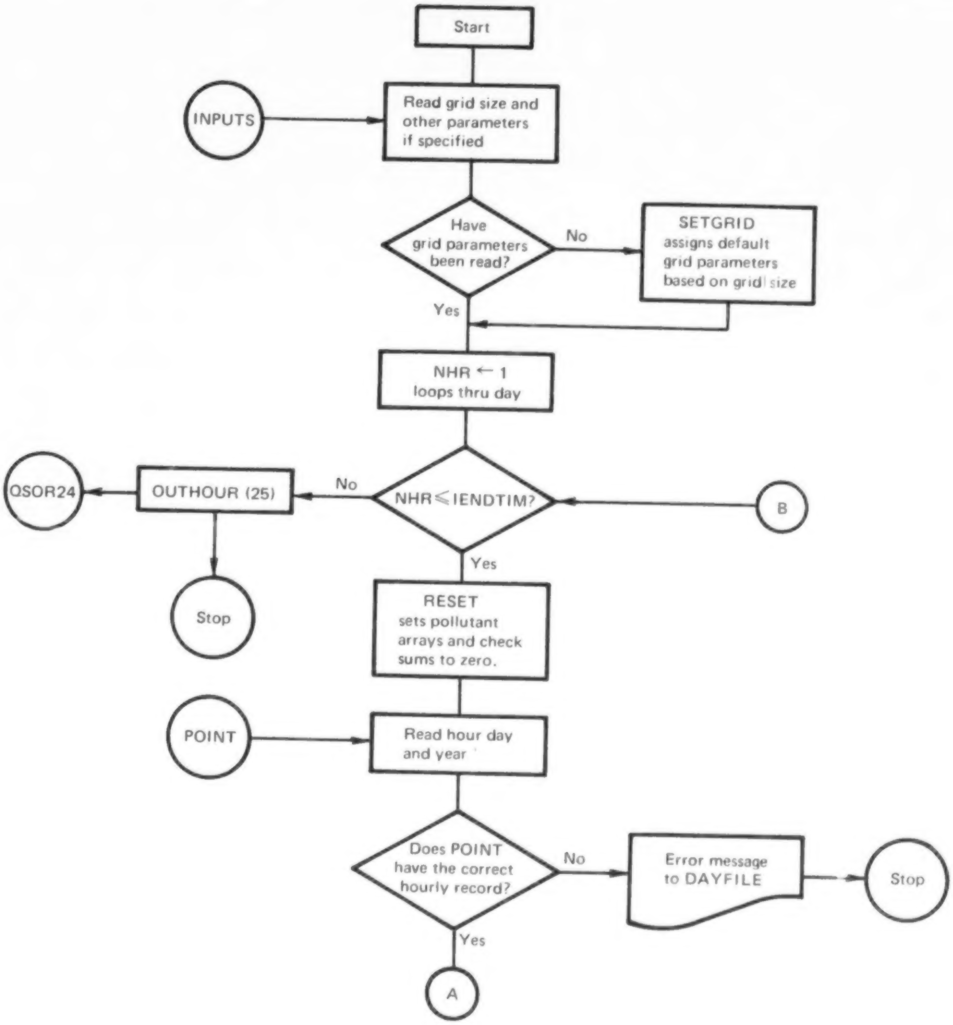

Start
INPUTS
Read grid size and other parameters if specified
Have grid parameters been read?
No
SETGRID assigns default grid parameters based on grid size
Yes
NHR ← 1 loops thru day
QSOR24
OUTHOUR (25)
No
NHR ≤ IENDTIM?
B
Stop
Yes
RESET sets pollutant arrays and check sums to zero.
POINT
Read hour day and year
Does POINT have the correct hourly record?
No
Error message to DAYFILE
Stop
Yes
A

FIGURE B-1. Source processor flowchart. Subroutine calls are indicated by a capitalized subroutine name in a process box.

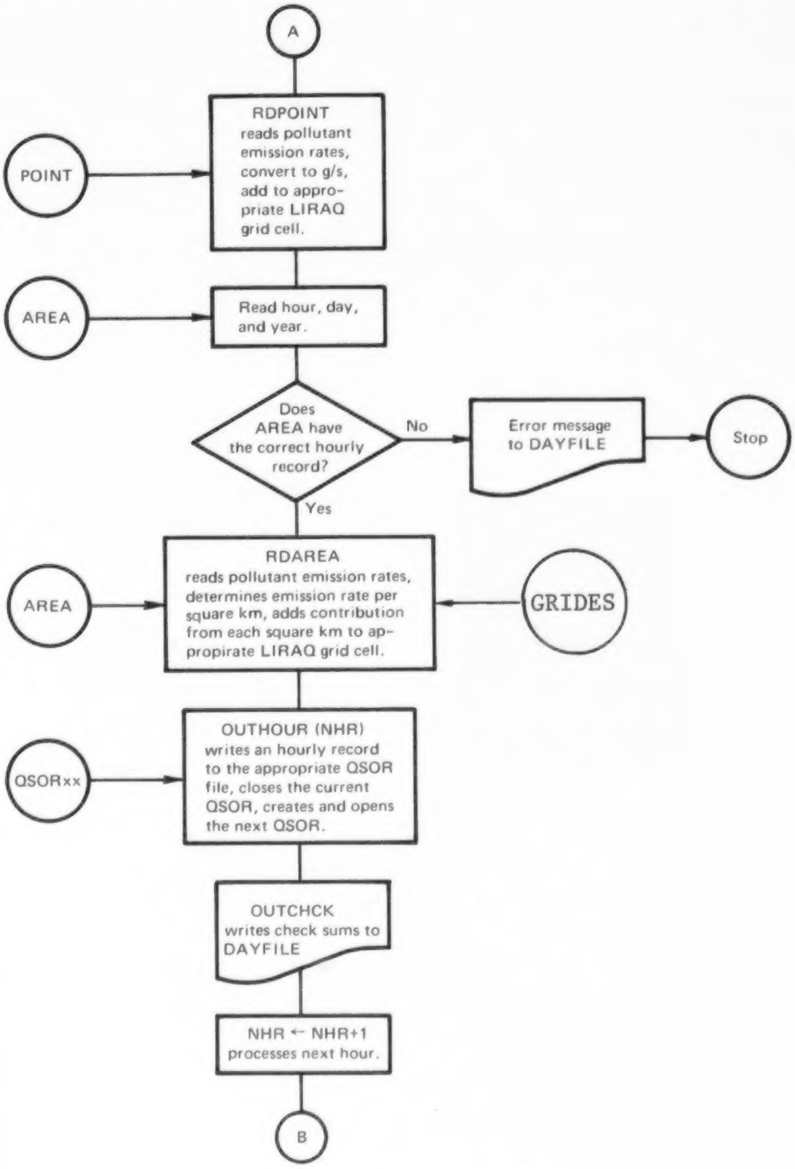

A
RDPOINT
reads pollutant
emission rates,
convert to g/s,
add to appro-
priate LIRAQ
grid cell.
POINT
AREA
Read hour, day,
and year.
Does
AREA have
the correct hourly
record?
No
Error message
to DAYFILE
Stop
Yes
RDAREA
reads pollutant emission rates,
determines emission rate per
square km, adds contribution
from each square km to ap-
propirate LIRAQ grid cell.
AREA
GRIDES
OUTHOUR (NHR)
writes an hourly record
to the appropriate QSOR
file, closes the current
QSOR, creates and opens
the next QSOR.
QSORxx
OUTCHCK
writes check sums to
DAYFILE
NHR ← NHR+1
processes next hour.
B

FIGURE B-1. Continued.

> "This file is logically broken into 24 units, one for each hour (00-23) of the day. A logical unit contains the following information. The first word is a 7 digit integer code for the data. The second word is the number of stacks which have emissions during this hour. The remaining words in a logical unit are divided into groups of 17 words. There will be a group of 17 words for each stack having emissions during this hour. At the end of the stack information the physical record is padded with zeros to complete the current 510 word record. The next physical record will contain data for the next logical unit (hour). Since the maximum number of stacks is 505, the maximum logical record size is 8587 words (2 + 17 * 505). There are a variable number of physical records for each logical record depending on the number of stacks for each hour."

The code CONVPT buffers in this binary data and writes out the information to file POINT in the BCD format described below.

The input file POINT contains all pollutant sources located at specific geographic points. The file contains data for one day with information presented in an hour-by-hour list. The lead card for each hourly data set is composed of the date and number of stacks in (I7, 2X, I5) format. The date is a decimal integer in the form yydddhh, where yy is the year, ddd is the Julian date, and hh is the hour of the day at which this hourly record begins. The hourly data sets are arranged in order. After the lead card there is one card for each point source. Each card contains fields for the following information:

UTM east coordinate (km)
UTM north coordinate (km)
Height (m)
Stack diameter (m)
Temperature (°C)
Flow rate (m x 10^3/min)
Emission rate of particulate (kg/h)
Emission rate of SO_x (kg/h)
Emission rate of NO_x (kg/h)
Emission rate of total hydrocarbon (kg/h)
Emission rate of CO (kg/h)
Emission rate of non-reactive hydrocarbon (moles/h)
Emission rate of paraffins (moles/h)
Emission rate of olefins (moles/h)
Emission rate of aromatics (moles/h)
Emission rate of aldehydes (moles/h)
Stack identification

These data are presented in the format (F7.2, F8.2, I4, F5.2, I4, F11.3, 5F11.3,/,39X,5F11.3,I12). An hourly data set is terminated by a negative value for the UTM east coordinate. The next card will be the lead card for the subsequent hour or an end of file if hour 2300 was just completed. Figure B-2 shows an example.

GRIDES

The input file GRIDES describes each RAPS grid cell. The information is read in binary form from the EPA/RAPS tape. The format of the binary data is described

```
7619500    358
 803.90 4284.10   4 0.    13       0.        10.356      0.         0.         0.         0.   
                                              0.         0.         0.         0.         0.     1414400104
 802.71 4278.69  24 1.22 398      57.765       .122       .165      3.116       .309       .847
                                             11.127       .371       .371       .124       .371  1414400201
 812.70 4275.10  12  .15 343       0.          .001       .003       .019       .002       .012
                                               .069       .002       .002       .001       .002  1414400401
 748.71 4305.63  76 4.72 164    2032.369      1.240      2.139     74.077       .189      2.100
                                              6.804       .227       .227       .076       .227  1446800101
 748.75 4305.60  76 5.18 148    2393.355      5.301    446.426    114.305      1.905      6.350
                                             68.583      2.286      2.286       .762      2.286  1446800102
 748.77 4305.58 106 4.57 144   12787.694     48.659   2276.771    582.957      9.716     32.386
                                            349.774     11.659     11.659      3.886     11.659  1446800103
 756.72 4290.88   9 2.32 485     176.841       .196       .353      2.577       .049       .074
                                              1.767       .059       .059       .020       .059  1446800201
 756.75 4290.89   9 2.32 485     176.841       .196       .353      2.577       .049       .074
                                              1.767       .059       .059       .020       .059  1446800202
 756.79 4290.90   9 2.32 485     176.841       .196       .353      2.577       .049       .074
                                              1.767       .059       .059       .020       .059  1446800203
 756.82 4290.91   9 2.32 485     176.841       .196       .353      2.577       .049       .074
                                              1.767       .059       .059       .020       .059  1446800204
 745.52 4283.13  72 4.11 165    5636.372     66.039    221.044    103.668      1.728      5.759
                                             62.201      2.073      2.073       .691      2.073  1446800307
 745.52 4283.15  72 4.11 165    5636.372     81.333    221.044    103.668      1.728      5.759
                                             62.201      2.073      2.073       .691      2.073  1446800308
 752.33 4304.55  48 3.63 198       0.        11.228    241.381     49.401      3.641      0.   
                                            131.072      4.369      4.369      1.456      4.369  1446800401
 752.34 4304.55  48 3.63 198       0.         5.963    147.296     27.500      2.143      0.   
                                             77.142      2.571      2.571       .857      2.571  1446800403
 752.36 4304.53  48 2.59 198       0.        10.842    205.660     45.875      3.213      0.   
                                            115.672      3.856      3.856      1.285      3.856  1446800405



                                              5.248       .175       .175       .058       .175  2643000903
 738.61 4268.09  21 1.83 209    1190.482       .039       .029     29.154       .146       .826
                                              5.248       .175       .175       .058       .175  2643000904
 738.61 4268.10  21 1.83 182     385.720       .373     33.910      6.480       .324       .432
                                             11.663       .389       .389       .130       .389  2643000905
 738.45 4268.20  40 1.22  76       0.          .196       .001      4.516       .059       .334
                                              2.121       .071       .071       .024       .071  2643000910
 738.45 4268.14  30 1.83  76       0.          .196       .001      4.516       .059       .334
                                              2.121       .071       .071       .024       .071  2643000911
 738.41 4268.14  37 1.83  76       0.          .002       .012      4.516       .059       .334
                                              2.121       .071       .071       .024       .071  2643000913
 738.46 4268.05  44 1.52  76       0.         0.       143.566      0.         0.         0.   
                                              0.         0.         0.         0.         0.     2643000916
 738.52 4268.02  60 1.83  82       0.         0.       113.668      0.         0.         0.   
                                              0.         0.         0.         0.         0.     2643000917
 732.62 4253.57  76 3.20 140    7746.504     52.525   2415.702    556.015      5.560     18.534
                                            200.166      6.672      6.672      2.224      6.672  2643001001
 732.67 4253.57  76 3.20 140    8154.215     55.289   2542.844    585.279      5.853     19.509
                                            210.701      7.023      7.023      2.341      7.023  2643001002
 732.72 4253.57 106 4.27 162   26318.656    144.127   6628.624   1525.692     15.257     50.856
                                            549.249     18.308     18.308      6.103     18.308  2643001003
 732.77 4253.57 106 4.72 162   26642.074    157.353   7236.905   1665.699     16.657     55.523
                                            599.651     19.988     19.988      6.663     19.988  2643001004
 737.16 4264.12  60 2.53 193      67.961       .108       .009      1.296       .086       .216
                                              3.107       .104       .104       .035       .104  2643001401
 734.43 4281.15  54 2.44 218     147.672     25.471     32.878      6.604       .440       .973
                                             15.850       .528       .528       .176       .528  2643001601
 718.84 4274.65   7  .34  33       0.         0.         0.         0.         2.088      0.   
                                              0.         0.        15.826      0.         0.     2643002001
 718.85 4274.65   7  .34  33       0.         0.         0.         0.          .870      0.   
                                              6.490      0.         0.         0.         0.     2643002002
 726.30 4273.55   4 0.    13       0.         0.         0.         0.          .217      0.   
                                               .673      2.243       .822      0.         0.     2643002901
 736.40 4262.50   9 0.    13       0.         0.         0.         0.        15.685      0.   
                                             48.624    162.183     59.446      0.         0.     2643003001
 710.80 4266.10   7 0.    13       0.         2.913      0.         0.         0.         0.   
                                              0.         0.         0.         0.         0.     2643003201
 710.80 4266.10   7 0.    13       0.         4.272      0.         0.         0.         0.   
                                              0.         0.         0.         0.         0.     2643003202
 710.80 4266.10   7 0.    13       0.         3.883      0.         0.         0.         0.   
                                              0.         0.         0.         0.         0.     2643003203
 710.80 4266.10   7 0.    13       0.        38.835      0.         0.         0.         0.   
                                              0.         0.         0.         0.         0.     2643003204
 736.80 4262.10   4 0.    13       0.       155.340      0.         0.         0.         0.   
                                              0.         0.         0.         0.         0.     2643003304
 -1.00
```

FIGURE B-2. Sample of POINT data. Several hundred pages of similar data have been omitted.

in a communication from EPA/RAPS as follows:

> "This file was created by inputting a UNIVAC record of 16001 words and adding 319 zero filled words on the end to force word boundary alignment after conversion of CDC format. This 16320 word buffer was then converted to CDC format and written to tape as 32 records of 510 CDC words each. The array containing the grid descriptions must be dimensioned (8,2000) to allow for a max of 2000 grid squares. The actual number of grid squares is currently fixed at 1989. The area source height and roughness height are both currently set to zero, but will be available at a later date."

The code CONVGD buffers in this binary data and writes out the information to file GRIDES in the BCD format described below.

The BCD file GRIDES contains one card for each RAPS grid cell. The file is read once as each hourly data set is processed. Each card contains fields for the following information:

Grid cell number
Area (km^2)
UTM east coordinate (km)
UTM north coordinate (km)
State number
County number
Source height (m)
Roughness height (m)

These data are presented in (2I7,2F12.3,2I10),2F12.3) format. The file terminates with a "-1" in columns 6,7. Figure B-3 is an example of this file.

AREA

The input file AREA contains all area sources for St. Louis. An area source is the total emission rate for one of the RAPS grid cells. The cells are square regions from one to ten kilometers on a side. The RAPS grid is irregular with small grid cells covering regions of high pollutant emission (to improve spatial resolution) and large grid cells covering regions which are minor pollutant sources. The file GRIDES describes the entire RAPS grid.

The data in the AREA file is first read in binary form from the EPA/RAPS tape. The format of the binary data is described in a communication from EPA/RAPS as follows:

> "This file was created by inputting a UNIVAC record of 22003 words (1 hour of data) and adding 337 zero filled words on the end to force word boundary alignment after conversion to CDC format. This 22440 word buffer was then converted to CDC format and written to tape as 44 records of 510 CDC words each. This was repeated for each of the 24 hours. The array containing the grid emissions must be dimensioned (11,2000) to allow for a max of 2,000 grids. The actual number of grid

```
   1   100    640.000   4235.000       26     1680     0.000      0.000
   2   100    640.000   4245.000       26     1680     0.000      0.000
   3   100    640.000   4265.000       26     1680     0.000      0.000
   4    25    640.000   4280.000       26     1680     0.000      0.000
   5    25    645.000   4230.000       26     1680     0.000      0.000
   6    25    645.000   4255.000       26     1680     0.000      0.000
   7    25    645.000   4260.000       26     1680     0.000      0.000
   8    25    645.000   4275.000       26     1680     0.000      0.000
   9    25    645.000   4280.000       26     1680     0.000      0.000
  10    25    650.000   4230.000       26     1680     0.000      0.000
  11   100    650.000   4235.000       26     1680     0.000      0.000
  12   100    650.000   4245.000       26     1680     0.000      0.000
  13   100    650.000   4255.000       26     1680     0.000      0.000
  14   100    650.000   4265.000       26     1680     0.000      0.000
  15    25    650.000   4275.000       26     1680     0.000      0.000
  16    25    655.000   4230.000       26     1680     0.000      0.000
  19   100    660.000   4235.000       26     1680     0.000      0.000
  20   100    660.000   4245.000       26     1680     0.000      0.000
  21   100    660.000   4255.000       26     1680     0.000      0.000
  22   100    660.000   4265.000       26     1680     0.000      0.000
  25    25    665.000   4230.000       26     1680     0.000      0.000
  26    25    670.000   4230.000       26     1680     0.000      0.000
  27   100    670.000   4235.000       26     1680     0.000      0.000
  28    25    670.000   4245.000       26     1680     0.000      0.000
  29    25    670.000   4250.000       26     1680     0.000      0.000
  32    25    670.000   4260.000       26     1680     0.000      0.000
  33     9    670.000   4265.000       26     1680     0.000      0.000
  34     1    670.000   4268.000       26     1680     0.000      0.000
  35     1    670.000   4269.000       26     1680     0.000      0.000
  37     1    671.000   4268.000       26     1680     0.000      0.000
  38     1    671.000   4269.000       26     1680     0.000      0.000
  39     1    672.000   4268.000       26     1680     0.000      0.000
  40     1    672.000   4269.000       26     1680     0.000      0.000
  43     1    673.000   4265.000       26     1680     0.000      0.000
  44     1    673.000   4266.000       26     1680     0.000      0.000
  45     1    673.000   4267.000       26     1680     0.000      0.000
  46     1    673.000   4268.000       26     1680     0.000      0.000
  47     1    673.000   4269.000       26     1680     0.000      0.000
  48     1    674.000   4265.000       26     1680     0.000      0.000
  49     1    674.000   4266.000       26     1680     0.000      0.000
  50     1    674.000   4267.000       26     1680     0.000      0.000
  51     1    674.000   4268.000       26     1680     0.000      0.000
  52     1    674.000   4269.000       26     1680     0.000      0.000
  53    25    675.000   4230.000       26     1680     0.000      0.000

2461     4    791.000   4228.000       14     6460     0.000      0.000
2462     4    793.000   4220.000       14     6460     0.000      0.000
2463     4    793.000   4222.000       14     6460     0.000      0.000
2464     4    793.000   4224.000       14     6460     0.000      0.000
2465     4    793.000   4226.000       14     6460     0.000      0.000
2466     4    793.000   4228.000       14     6460     0.000      0.000
  -1
```

FIGURE B-3. Sample of GRIDES input. Many similar lines have been omitted.

> squares is currently fixed at 1989. The grid emissions are output is ascending order by grid number."

The code CONVAR buffers in this binary data and writes out the information to file AREA in the BCD format described below.

The file contains data for one day with the information presented in an hour-by-hour list. The lead card for each hourly data set is composed of the date and hour in (2I7) format. The hours range from 0 to 23 in order. The date is a decimal integer in the form yyddd, where yy is the year, and ddd is the Julian date. After the lead card there is one card for each RAPS grid square with a nonzero emission rate for some pollutant. The cards for each grid square are in the same order as the cards in the file GRIDES; consequently, the first card after the hourly lead card in AREA gives the area emission rates for the grid cell described by the first card in GRIDES, and so on through the files. Each card contains fields for the following information:

Emission rate of particulate (kg/h)
Emission rate of SO_x (kg/h)
Emission rate of NO_x (kg/h)
Emission rate of total hydrocarbon (kg/h)
Emission rate of CO (kg/h)
Emission rate of dust (kg/h)
Emission rate of non-reactive hydrocarbon (moles/h)
Emission rate of paraffins (moles/h)
Emission rate of olefins (moles/h)
Emission rate of aromatics (moles/h)
Emission rate of aldehydes (moles/h)

These data are in (11F10.2) format. The maximum emission rate for any one square are checked against the following values (based on advice from EPA). These values can easily be modified.

SO_x	49.94 kg/h
Suspended particulate	600.00
NO_x	337.78
Total Hydrocarbon	269.14
CO	1443.81

An hourly data set is terminated by a negative particulate rate value. The next card will be the lead card for the next hour or an end of file if hour 23 was just completed. Figure B-4 is an example of this.

INPUTS

INPUTS is a small control file. Normally only the LIRAQ grid cell size is read from this file. However, several quantities can be changed from the default values that are used if desired. This file is read by a NAMELIST command as described in the CDC FTN4 manual. Thus, one can change one set of variables without putting in values for all previously read variables. Below, in Table B-1, the variable with the default and description are presented. If a nonstandard grid is to be used (i.e., a grid other than 1, 2, 3, 4, or 5 km on a side) all NAMELIST variables associated with grid specifications must be defined in input since no default values will have been defined. Non-standard grids must be square grids with integral dimensions (e.g. 6 x 6, 7 x 7, 10 x 10, 20 x 20). Figure B-5 gives a sample input file.

OUTPUT FILES

Each QSOR file contains emissions data for a one hour period, thus SORP generates 24 QSORs (QSOR00 to QSOR23) from the input data. QSOR24 contains the same information as QSOR23. LIRAQ deals with two types of pollutant sources; elevated sources are taken to be those emitted at a height of 20 m or more, while surface sources are those emitted closer to the surface. Elevated sources are listed first in all QSOR files. Any LIRAQ grid cell containing a nonzero elevated emission

```
76195    0
   74.54        .00        .16        .15        .08       0.         1.28       1.31        .55        .01        .03
   85.44        .36       3.39       3.60      24.87       1.75      10.74      21.81      14.35       5.06       3.91
   71.52        .01        .58        .38       2.15        .14       2.54       2.40       1.46        .43        .31
   13.77        .74       5.09       1.48       1.68       0.         2.52       4.21       4.19        .87       4.34
   14.79        .00        .16        .09        .07       0.         1.04        .73        .32        .01        .03
   14.63        .00        .06        .01        .03       0.          .32        .02        .03        .00        .01
   18.66        .00        .06        .01        .03       0.          .32        .02        .03        .00        .01
   12.68        .38       2.94       1.61       9.19        .61       3.66       6.49       5.74       2.14       3.24
   20.30        .41       3.19       1.12       1.02       0.         3.23       5.32       3.41        .48       2.38
    9.56        .00        .24        .04        .11       0.         1.25        .07        .11        .01        .04
   84.19        .01        .37        .31       2.30        .16       2.13       1.68       1.23        .45        .31
   68.75        .42       3.53       3.05      23.88       1.67       8.66      16.30      12.16       4.86       3.95
   75.06        .01        .80        .71       2.11        .14       4.33       5.66       2.65        .41        .32
   63.14        .71       6.96       4.52      20.33       1.35      15.00      25.91      16.43       4.58       6.30
    8.77        .72       4.92       1.37       1.65       0.         2.14       3.38       3.81        .85       4.22
   10.36        .03       1.05       1.09       7.14        .61       4.23       6.59       4.40       1.45       1.04
   68.73        .80      13.34      11.60      80.24       7.15      32.08      62.83      46.65      16.82      14.17
   55.48        .29       2.85       2.68      26.20       1.30       8.16      13.55      11.17       4.49       3.71
   66.06        .19       2.33       2.19      15.66        .79       8.48      13.61       8.80       2.72       2.31
   60.39       1.50      11.65       5.40      26.99       1.71      14.46      20.95      18.66       6.46      11.37
   16.25        .05       2.58       2.33      15.04       1.04      14.44      13.92       9.12       3.00       2.11
   14.69       0.          .04        .01        .02       0.          .22        .01        .02        .00        .01
   63.66        .53       8.56       8.19      50.83       4.39      24.72      48.32      32.60      10.64       9.02
   15.20        .09       2.19       1.96      14.66       1.31       6.37      10.37       8.02       3.03       2.31
   16.13        .00        .24        .09        .14       0.         1.59        .53        .32        .02        .05
    7.17        .04       1.25       1.70      15.01       1.08       6.52       8.97       7.02       3.03       1.94
    2.29        .00        .20        .22       1.58        .11       1.28       1.29        .89        .31        .21
     .25       0.          .04        .01        .03       0.          .28        .02        .03        .00        .01
     .27        .01        .18        .26       2.33        .17        .94       1.32       1.06        .47        .30
     .25       0.          .04        .03        .03       0.          .34        .20        .10        .00        .01
     .27        .01        .18        .27       2.28        .16        .98       1.47       1.11        .46        .29
     .26        .01        .10       5.78        .35        .02      29.52      38.54       1.60      12.82        .83
     .27        .01        .18        .42       2.29        .17       1.46       3.07       1.69        .46        .30
     .26        .01        .18        .28       2.58        .19        .86       1.46       1.16        .52        .33
     .26        .01        .17        .27       2.53        .18        .84       1.43       1.14        .51        .32
     .26        .01        .18        .29       2.53        .18        .91       1.61       1.21        .51        .32
     .30        .02        .52        .96       8.04        .47       2.96       5.84       4.00       1.46        .97
     .29        .17        .41       1.69       2.63        .13       7.86      11.22       1.96       3.30        .60
     .24       0.          .02        .00        .01       0.          .12        .01        .01        .00        .00
     .24       0.          .02        .00        .01       0.          .12        .01        .01        .00        .00
     .24       0.          .02        .00        .01       0.          .12        .01        .01        .00        .00
     .29        .03        .55        .90       7.72        .39       2.83       5.48       3.78       1.32        .97
     .36        .15       1.26        .83       3.91        .26       2.16       4.46       3.01        .89       1.28
   16.30       0.          .04        .01        .02       0.          .22        .01        .02        .00        .01
   17.24        .12       3.94       4.29      35.42       2.98      13.54      22.53      17.79       7.24       4.97
   16.43        .25       3.00       3.25      31.28       1.63      10.91      16.89      13.62       5.46       4.22
   18.03        .00        .32        .07        .18       0.         1.94        .11        .20        .02        .07
    9.37       1.01       7.35       5.22      38.04       1.84      14.36      25.61      20.14       7.07       8.48
  119.02        .00        .17        .07        .08       0.         1.05        .49        .25        .01        .03
  137.51        .79      17.14      18.73     127.32      11.20      52.78     106.89      75.73      26.65      21.05
   16.88       0.          .04        .01        .02       0.          .22        .01        .02        .00        .01
   71.23        .09       2.12       3.37      30.92       2.25      10.29      17.94      14.06       6.25       3.92
   78.27        .76       8.98       6.07      38.95       3.39      17.24      30.35      23.61       8.38       8.71
   42.26       1.92      29.12      25.71     200.84      14.89      72.36     135.69     104.57      39.26      32.97
   13.08        .71       5.39       2.65      16.06        .74       5.98      10.53       9.50       3.26       5.61
   28.38        .05        .52        .91       3.93        .28       3.00       7.16       3.59        .78        .54
   27.19       0.          .08        .97        .04       0.         3.39       9.97       3.68        .00        .01
   36.72       0.          .08        .49        .04       0.         1.90       5.00       1.86        .00        .01
   17.65        .01        .33        .56       4.84        .35       1.75       3.19       2.34        .97        .61
   16.36       1.02       7.33       2.19       2.75       0.         4.31       9.12       6.56       1.06       5.25
   25.19        .13       1.13        .53       3.92        .26       1.64       2.35       2.00        .81        .90
```

FIGURE B-4. Sample of AREA source data. Several pages of similar data have been omitted.

TABLE B-1. INPUTS file description.

Variable	Default and description
IGRIDSZ	No default. This variable must be specified. It is the length of the side of a LIRAQ grid cell and must be an integer from 1 to 5.
LUTMEO, LUTMNO	LUTMEO is the UTM east coordinate (km) and LUTMNO is the UTM north coordinate (km) of the southwest corner of the LIRAQ grid. LUTMEO and LUTMNO must be integers. The defaults depend on the size of the LIRAQ grid cells. Default values are: IGRIDSZ LUTMEO LUTMNO 1 654 4213 2 654 4214 3 654 4215 4 656 4216 5 655 4215
JMXE, IMXN	JMXE is the number of LIRAQ grid cells along the east axis; IMXN is the number of LIRAQ grid cells along the north axis. JMXE and IMXN must both be integers. The defaults depend on the size of the LIRAQ grid cells. Defaults are: IGRIDSZ JMXE IMXN 1 159 117 2 79 58 3 53 38 4 39 28 5 31 23
AC2C, AC1C, ARCHO, PC2C, PC1C, PRCHO	These variables were used to split the hydrocarbon emission rates available in the NEDS input into the pollutant species that LIRAQ requires. Different constants are required for area and point sources. These variables are real numbers. Defaults are: AC2C (area alkenes) 0.77 AC1C (area alkanes) 0.24 ARCHO (area aldehydes) 0.06 PC2C (point alkenes) 0.73 PC1C (point alkanes) 0.20 PRCHO (point aldehydes) 0.035

TABLE B-1. Continued.

Variable	Default and description
IENDTIM	Specifies the end of the time period to be processed, i.e., it is one more than the beginning of the last hourly data set to be examined. If IENDTIM is < 24, then a copy of the last QSOR is not generated. It should be an integer from 1 to 24. The default is 24.
NEDS	NEDS is set to one if a diurnal variation in pollutant emissions is desired when NEDS area sources are used. Default is zero.
FACCO, FACHC, FACNOX, FACSOX	These variables are used to implement diurnal variation in pollutant emission rates for area sources if NEDS is set to one. These variables are arrays dimensioned 24, one value for each hour. The value for a given hour is multiplied by the input emission rate for a pollutant to vary otherwise constant NEDS data. Particulate data are not varied. For the other pollutants default values are:

Pollutant:	CO	hydrocarbon	NO_x	SO_x
Array name:	FACCO	FACHC	FACNOX	FACSOX
hour: 0	0.234	0.204	0.368	0.670
1	0.151	0.165	0.227	0.670
2	0.089	0.138	0.165	0.670
3	0.048	0.120	0.124	0.670
4	0.089	0.138	0.165	0.670
5	0.089	0.138	0.165	0.670
6	0.426	0.524	0.463	0.698
7	1.415	0.953	1.274	0.698
8	1.587	1.946	1.452	1.488
9	0.903	1.653	0.950	1.488
10	1.111	1.745	1.155	1.488
11	1.298	1.828	1.322	1.488
12	1.381	1.865	1.420	1.488
13	1.277	1.819	1.318	1.488
14	1.485	1.911	1.522	1.488
15	1.838	2.068	1.870	1.488
16	2.088	2.164	1.884	1.488
17	1.997	1.199	1.733	0.922
18	1.482	0.790	1.543	0.734
19	1.627	0.855	1.686	0.734
20	1.521	0.615	1.156	0.743
21	0.857	0.513	0.931	0.734
22	0.587	0.360	0.655	0.670
23	0.421	0.286	0.492	0.670

```
$SOR
IGRIDSZ = 5.
NEDS = 1.
$
```

FIGURE B-5. Sample of file INPUTS.

rate is included in the list with one card containing the data for one grid cell. Following the elevated sources the surface sources are listed in a similar manner. Each card in these lists contains the UTM coordinates of the grid cell and emission rates in g/s for the seven pollutants required by LIRAQ. Zero values for both UTM coordinates terminate the current set of elevated or surface source data. The card format and information are shown in Table B-2. Figure B-6 gives an example of QSOR.

TABLE B-2. Card formats and information for QSOR file.

Card no.	Card format	Information
1	(18X,I2,35X,2A10)	Number of pollutants, format for subsequent data cards. There are two cards in this format at the beginning of QSOR00. These cards determine how data for a grid cell is to be input. The first card indicates the format for elevated source data; the second card indicates the format for surface source data.
2	(54X,I3,3X,I3)	This card specifies the period of time for which the data in this QSOR file are valid. The two values are the beginning and ending times of the period. This card is the first card in all QSOR files except QSOR00.
3	(A10)	The elevated source data are started with an "ELEVATED SOURCE DATA" card.
4	(1X,I4,I5,7310.3)	UTM east coordinate (km), UTM north coordinate (km), emission rates for particulates, alkanes, alkenes, aldehydes, nitric oxide, sulfur dioxide, and carbon monoxide in g/s. This format is specified in the first two fields terminate the data set.
5	(A10)	The surface source data are begun with a "SURFACE SOURCE DATA" card. The data are in the same format at the elevated source data.

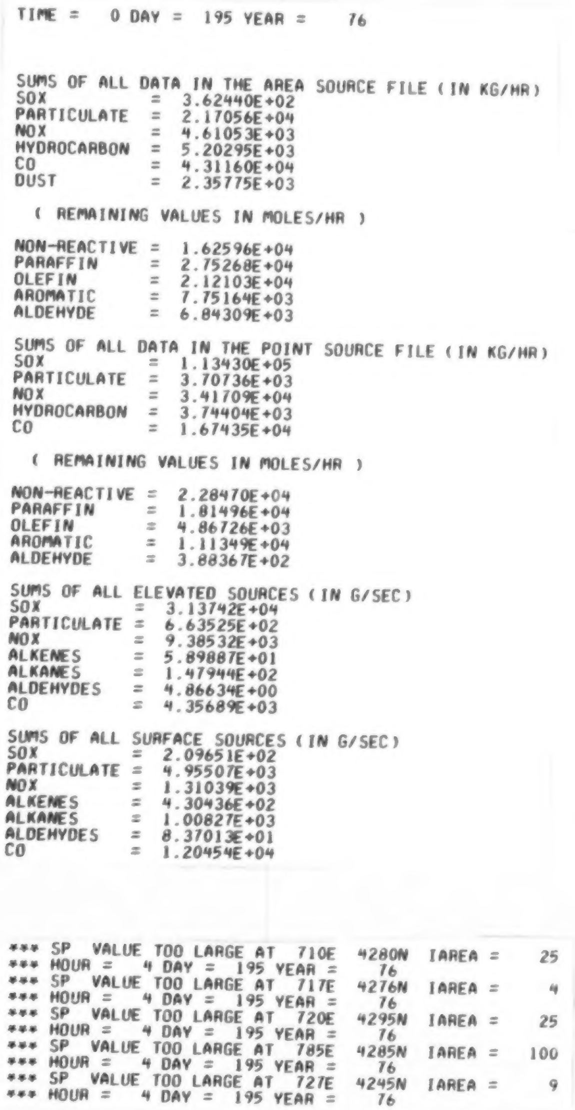
```
INPUT FORMAT FOR  7 COLUMNS OF ELEVATED SOURCE DATA   (1X,I4,I5,7E10.3)
INPUT FORMAT FOR  7 COLUMNS OF  SURFACE SOURCE DATA   (1X,I4,I5,7E10.3)
THE FOLLOWING DATA SET IS VALID BETWEEN THE HOURS OF   0 TO   1     197 1975
ELEVATED SOURCE DATA
 775 4230 4.082E+01 5.122E+00 1.870E+01 8.964E-01 3.645E+03 9.665E+03 8.536E+01
 730 4250 4.566E+01 1.128E+00 4.116E+00 1.974E-01 5.647E+02 1.566E+03 1.883E+01
 735 4260 3.056E-02 5.556E-03 2.028E-02 9.722E-04 3.611E-01 2.778E-03 5.556E-02
 775 4260 5.694E-01 2.222E-02 8.111E-02 3.889E-03 3.111E+00 1.444E+01 3.056E-01
 720 4265 7.222E-02 0.        0.        0.        4.500E+00 5.556E-03 1.111E-01
 730 4265 3.678E+00 0.        0.        0.        3.508E+01 1.335E+01 0.
 735 4265 9.617E+00 2.222E-01 8.111E-01 3.889E-02 2.964E+01 1.681E+02 2.056E+00
 760 4265 1.205E+01 1.111E-02 4.056E-02 1.944E-03 1.472E+00 8.694E+00 8.333E-02
 685 4270 7.180E+01 5.689E+00 2.076E+01 9.956E-01 2.847E+03 1.021E+04 9.489E+01
 740 4270 6.528E+00 5.556E-01 2.028E+00 9.722E-02 3.722E+00 4.650E+00 6.511E+01
 735 4275 1.144E+01 3.333E-02 1.217E-01 5.833E-03 2.444E+00 1.481E+01 3.611E-01
 740 4275 6.944E-01 4.444E-02 1.622E-01 7.778E-03 2.089E+01 1.504E+01 8.333E-01
 745 4275 0.        0.        0.        0.        4.194E+00 7.317E+01 0.
 800 4275 3.333E-02 1.667E-02 6.083E-02 2.917E-03 8.611E-01 4.722E-02 2.500E-01
 730 4280 7.075E+00 2.222E-02 8.111E-02 3.889E-03 1.833E+00 9.133E+00 2.778E-01
 735 4280 3.250E-01 7.222E-02 2.636E-01 1.264E-02 5.583E+00 4.096E+01 7.500E-01
 740 4280 1.758E+01 6.056E-01 2.210E+00 1.060E-01 1.914E+01 2.976E+01 6.597E+01
 745 4280 5.649E+01 2.444E-01 8.922E-01 4.278E-02 7.483E+01 1.101E+02 3.833E+00
 745 4285 5.278E-01 1.667E-02 6.083E-02 2.917E-03 2.944E+00 2.778E+00 2.222E-01
 725 4290 7.778E-02 0.        0.        0.        1.889E+00 0.        1.111E-01
 730 4290 6.944E-02 0.        0.        0.        1.528E+00 0.        8.333E-02
 740 4290 1.836E+02 0.        0.        0.        7.008E+01 2.666E+01 0.
 785 4290 9.222E+00 1.000E-01 3.650E-01 1.750E-02 7.083E+00 5.910E+01 1.056E+00
 750 4300 7.922E+01 5.256E+00 1.918E+01 9.197E-01 7.794E+01 1.362E+03 1.340E+03
 755 4300 0.        0.        0.        0.        0.        4.033E+00 0.
 740 4305 1.111E-02 0.        0.        0.        5.556E-02 1.667E-02 0.
 745 4305 3.531E+01 1.361E+00 4.968E+00 2.382E-01 4.302E+02 2.469E+03 2.283E+01
 730 4310 2.008E+00 1.094E+00 3.995E+00 1.915E-01 1.004E+03 2.302E+03 1.825E+01
   0    0
SURFACE SOURCE DATA
 655 4230 6.833E-01 9.357E-02 3.002E-01 2.339E-02 5.367E-01 3.666E-01 2.400E+00
 655 4235 2.597E-01 6.491E-02 2.082E-01 1.623E-02 3.864E-01 1.214E-01 1.696E+00
 655 4240 2.597E-01 6.491E-02 2.082E-01 1.623E-02 3.864E-01 1.214E-01 1.696E+00
 655 4245 3.042E-01 5.617E-02 1.802E-01 1.404E-02 3.690E-01 1.638E-01 1.423E+00
 655 4250 3.042E-01 5.617E-02 1.802E-01 1.404E-02 3.690E-01 1.638E-01 1.423E+00
 655 4255 4.382E-01 4.332E-02 1.390E-01 1.083E-02 2.405E-01 2.410E-01 1.096E+00
 655 4260 4.382E-01 4.332E-02 1.390E-01 1.083E-02 2.405E-01 2.410E-01 1.096E+00
 655 4265 5.750E-01 4.627E-02 1.485E-01 1.157E-02 3.005E-01 3.308E-01 1.115E+00
 655 4270 5.750E-01 4.627E-02 1.485E-01 1.157E-02 3.005E-01 3.308E-01 1.115E+00
 660 4230 5.261E+00 2.776E-01 8.906E-01 6.939E-02 1.496E+00 3.047E+00 6.607E+00
 660 4235 4.590E-01 4.525E-02 1.452E-01 1.131E-02 2.908E-01 2.638E-01 1.109E+00
 660 4240 4.590E-01 4.525E-02 1.452E-01 1.131E-02 2.908E-01 2.638E-01 1.109E+00
 660 4245 2.729E-01 6.168E-02 1.979E-01 1.542E-02 3.854E-01 1.373E-01 1.593E+00
 660 4250 2.729E-01 6.168E-02 1.979E-01 1.542E-02 3.854E-01 1.373E-01 1.593E+00
 660 4255 2.681E-01 6.208E-02 1.992E-01 1.552E-02 3.884E-01 1.317E-01 1.607E+00
 805 4260 1.000E-01 3.444E-02 1.105E-01 8.610E-03 1.574E-01 5.816E-02 9.373E-01
 805 4265 1.236E-01 3.533E-02 1.133E-01 8.831E-03 1.623E-01 6.514E-02 9.121E-01
 805 4270 1.236E-01 3.533E-02 1.133E-01 8.831E-03 1.623E-01 6.514E-02 9.121E-01
 805 4275 2.097E-01 4.794E-02 1.538E-01 1.199E-02 1.998E-01 1.214E-01 1.087E+00
 805 4280 2.097E-01 4.794E-02 1.538E-01 1.199E-02 1.998E-01 1.214E-01 1.087E+00
 805 4285 9.444E-02 3.587E-02 1.151E-01 8.967E-03 1.720E-01 4.560E-02 1.039E+00
 805 4290 9.444E-02 3.587E-02 1.151E-01 8.967E-03 1.720E-01 4.560E-02 1.039E+00
 805 4295 8.958E-02 3.417E-02 1.096E-01 8.542E-03 1.689E-01 4.932E-02 8.476E-01
 805 4300 8.958E-02 3.417E-02 1.096E-01 8.542E-03 1.689E-01 4.932E-02 8.476E-01
 805 4305 6.167E-01 1.416E-01 4.543E-01 3.540E-02 4.695E-01 4.713E-01 2.773E+00
 805 4310 6.167E-01 1.416E-01 4.543E-01 3.540E-02 4.695E-01 4.713E-01 2.773E+00
 805 4315 9.167E-02 3.329E-02 1.068E-01 8.321E-03 1.602E 01 5.444E-02 8.027E-01
 805 4320 9.167E-02 3.329E-02 1.068E-01 8.321E-03 1.602E-01 5.444E-02 8.027E-01
 805 4325 1.533E+00 9.361E-01 3.003E+00 2.340E-01 5.483E+00 3.592E-01 2.590E+01
   0    0
```

FIGURE B-6. Example of a 5-km QSORxx file. This is QSOR00 and the first two lines appear in this file only; otherwise, this file is typical of all QSOR files. A large number of lines in the surface-source section have been omitted.

DAYFILE

Checksums for each hour's input and output are computed and written to the DAYFILE. The first two sets of checksums give the total emissions read from the files AREA and POINT, respectively, in kg/h. The last two sets of checksums are the totals of all elevated source data and surface source data, respectively, written to the QSOR file for an hour. These sums are in g/s. Also, if any input values from the file AREA are larger than the specified limits, a warning is sent to the DAYFILE.

See Fig. B-7 for an example of the checksum output.



```
TIME =   0 DAY =  195 YEAR =    76


SUMS OF ALL DATA IN THE AREA SOURCE FILE ( IN KG/HR)
SOX           =  3.62440E+02
PARTICULATE   =  2.17056E+04
NOX           =  4.61053E+03
HYDROCARBON   =  5.20295E+03
CO            =  4.31160E+04
DUST          =  2.35775E+03

  ( REMAINING VALUES IN MOLES/HR )

NON-REACTIVE =  1.62596E+04
PARAFFIN     =  2.75268E+04
OLEFIN       =  2.12103E+04
AROMATIC     =  7.75164E+03
ALDEHYDE     =  6.84309E+03

SUMS OF ALL DATA IN THE POINT SOURCE FILE ( IN KG/HR)
SOX           =  1.13430E+05
PARTICULATE   =  3.70736E+03
NOX           =  3.41709E+04
HYDROCARBON   =  3.74404E+03
CO            =  1.67435E+04

  ( REMAINING VALUES IN MOLES/HR )

NON-REACTIVE =  2.28470E+04
PARAFFIN     =  1.81496E+04
OLEFIN       =  4.86726E+03
AROMATIC     =  1.11349E+04
ALDEHYDE     =  3.88367E+02

SUMS OF ALL ELEVATED SOURCES ( IN G/SEC)
SOX          =  3.13742E+04
PARTICULATE =  6.63525E+02
NOX          =  9.38532E+03
ALKENES      =  5.89887E+01
ALKANES      =  1.47944E+02
ALDEHYDES    =  4.86634E+00
CO           =  4.35689E+03

SUMS OF ALL SURFACE SOURCES ( IN G/SEC)
SOX          =  2.09651E+02
PARTICULATE =  4.95507E+03
NOX          =  1.31039E+03
ALKENES      =  4.30436E+02
ALKANES      =  1.00827E+03
ALDEHYDES    =  8.37013E+01
CO           =  1.20454E+04



*** SP  VALUE TOO LARGE AT  710E  4280N  IAREA =    25
*** HOUR =   4 DAY =  195 YEAR =    76
*** SP  VALUE TOO LARGE AT  717E  4276N  IAREA =     4
*** HOUR =   4 DAY =  195 YEAR =    76
*** SP  VALUE TOO LARGE AT  720E  4295N  IAREA =    25
*** HOUR =   4 DAY =  195 YEAR =    76
*** SP  VALUE TOO LARGE AT  785E  4285N  IAREA =   100
*** HOUR =   4 DAY =  195 YEAR =    76
*** SP  VALUE TOO LARGE AT  727E  4245N  IAREA =     9
*** HOUR =   4 DAY =  195 YEAR =    76
```

FIGURE B-7. Sample of checksum output. Many lines of similar output have been omitted.

APPENDIX C

GRAPHIC DISPLAY OF REGIONAL AIR MONITORING SYSTEM DATA

This appendix describes a graphic processor, UADATA, which helps the user analyze meteorological data. Specifically, the program displays, for user-selected data times (edit hours), the surface wind speed and direction, temperature, dew point, incident solar radiation, and vertical profiles of wind speed and direction. These displays are in the form of two- and three-dimensional plots overlaid with some reference information (i.e., a map grid, topographic features, and a user-defined grid). The program was written to assist in evaluating meteorological data from the St. Louis study conducted by the Environmental Protection Agency (EPA).

The input to the program consists of the following binary coded decimal (BCD) files:

RAMS - The surface and upper air data from the Regional Air Monitoring System.

RAPS - The Regional Air Pollution Study grid.

RIV - River outline segments from the St. Louis area.

INPUT - A list of edit hours, controlling the amount of data displayed, (00 to 23, with a -01 terminator, Format 25I2).

A more complete description is provided in Stullich et al. (1978).

DESCRIPTION OF RAMS FILE

An information file (20A4) is the first file of a five-file tape. This tape contains the meteorological (both upper air and surface) and pollutant measurement data for four days of 1975: 191 (July 10), 195 (July 14), 197 (July 16), and 231 (August 19). The data for each day are presented on a separate file in that order.

Upper Air Data

The upper air data (UAD), consisting of either pilot balloon (pibal) or radiosonde data, are presented for an entire 24 h at the beginning of each day. The lead card contains a variable indicator (IND), the time of release, day, year, and station. These fields are in the format (I2,I5,I4,I5,I4). IND is 80 (pibal), 81 (radiosonde), or 89 (end of upper air data). IND 82 indicates radiosonde without wind data, i.e., wind speed and direction = 0. Time is given by hour and minute. Stations 141, 142, 143 and 144 are possible release points.

Behind each lead card are data cards containing the data list corresponding to the balloon release. The data include height (m above mean sea level), wind speed (m/s), direction (deg az), pressure (mbar), temperature (^{o}C), potential temperature (K), dew point (^{o}D), mixing ratio (g/kg), and saturation mixing ratio (g/kg). The format is 20X, 9F6.1. The last six values are applicable only to radiosondes (IND = 81 or 82). The value -100 for either wind speed or direction signifies missing data. The program terminates the reading of data for each release when it encounters a negative height. The reading of UAD for the day terminates when the program encounters IND = 89.

Surface Data

An hour-by-hour list of surface data from the RAMS network follows the upper air data. The lead card contains a variable indicator, hour, day, and year. The format for these fields if (I2,I5,I4,I5). The hour represents the 60 minutes starting at the given Central Standard Time (CST). The variable indicators are defined in Table C-1.

A set of 25 numbers corresponding to RAMS stations 101-125 follows each lead card. The format is (20X,5E12.5). At each hour, starting at hour zero, and continuing through hour 23, the program writes for all 22 variables. After reading variable 31 of hour 23, an IND = 99 appears, followed by an end-of-file message. A data flag 1.E+37 indicates missing data. An hour must have more than 15 minutes of data or data are classified as missing. The value 1.E+14 indicates an outlier data point. Generally, anything greater than 1.E+7 is special (flagged) data.

DESCRIPTION OF RAPS FILE

The RAPS file contains data describing the Regional Air Pollution Study grid. The file lists several data triplets which delineate the lower left (i.e., southwest) corner of each square subzone in UTM coordinates (km) and the area of that subzone. The format is 5(4X,I3,I4,I3,1X).

DESCRIPTION OF RIV FILE

The RIV file contains river outline segments from the St. Louis area. Segments, delimited between *BEGINSEG cards, consist of lists of UTM coordinate pairs. The format is (1X,6(F6.0,F7.0)).

The processor produces 35-mm film plots for each hour of each day desired. Table C-2 describes the plots available. Sample plots generated from actual data are given in the microfiche addendum to this report.

TABLE C-1. Variable indicators for lead cards containing surface data in the RAMS file.

Variable	Indicator	Units
Wind speed	WS	m/s
Wind direction	WD	deg clockwise from north
Temperature	T	°C
Dew point	DP	°C
Barometric pressure	BP	mbar
Temperature difference	DT	°C (difference between 30-m level and 6-m level)
Pyranometer	PYRA(1)	Langleys/min, all wave lengths
Pyranometer	PYRA(2)	Langleys/min, greater than 3950 Å
Pyranometer	PYRA(3)	Langleys/min, greater than 6950 Å
Pyrgeometer	PYRG	Langleys/min
Ozone	O_3	ppm by vol
Carbon monoxide	CO	ppm by vol
Methane	CH_4	ppm by vol
Total hydrocarbons	THC	ppm by vol (carbon)
Nitric oxide	NO	ppm by vol
Nitrogen dioxide	NO_2	ppm by vol
Oxides of nitrogen	NO_x	ppm by vol
Total particulate sulfur	TS	ppm by vol
Hydrogen sulfide	H_2S	ppm by vol
Sulfur dioxide	SO_2	ppm by vol
Nephelometer	NEPH(1)	m^{-1}
Nephelometer	NEPH(2)	m^{-1}

TABLE C-2. Plots of raw meteorological data.

Figure	Description
C-1	St. Louis RAMS and UAD station locations.
C-2	St. Louis RAPS grid.
C-3	A three-dimensional plot showing variation of horizontal wind speed and direction (both surface and upper air).
C-4	A plot like C-3, but rotated 90° clockwise in the X,Y plane.
C-5	A three-dimensional plot showing total incident solar radiation.
C-6	A plot like C-5, but showing only wavelengths less than 3950 Å.
C-7	A plot like C-5, but showing only wavelengths greater than 6950 Å.
C-8	A two-dimensional, horizontal plot of surface temperature.
C-9	A two-dimensional, horizontal plot of surface winds.
C-10	A vertical, scalar plot of upper air station data including temperature, dew point, wind speed, and direction.

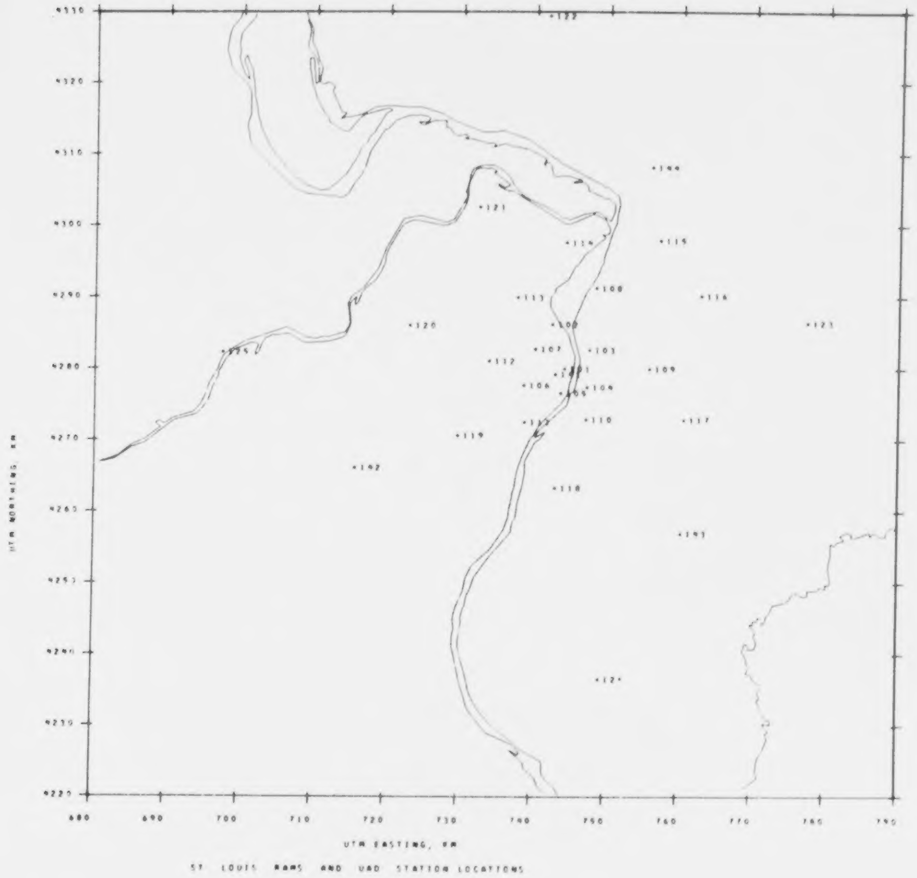

4330
4320
4310
4300
4290
4280
4270
4260
4250
4240
4230
4220
UTM NORTHING, KM
680
690
700
710
720
730
740
750
760
770
780
790
UTM EASTING, KM
ST. LOUIS RAMS AND UAD STATION LOCATIONS
122
144
121
114
115
108
113
116
120
102
123
125
107
103
112
101
109
106
104
105
111
110
117
119
142
118
143
124

FIGURE C-1. Locations of St. Louis RAMS and UAD stations.

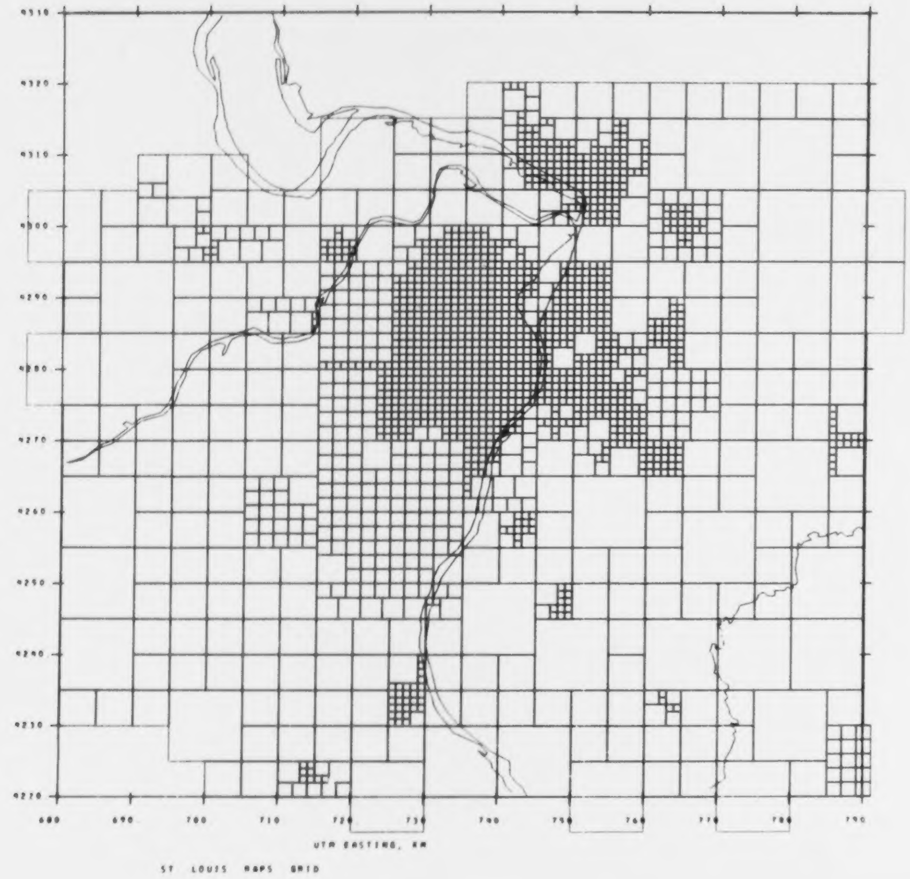

4330
4320
4310
4300
4290
4280
4270
4260
4250
4240
4230
4220
UTM NORTHING, KM
680
690
700
710
720
730
740
750
760
770
780
790
UTM EASTING, KM
ST LOUIS RAPS GRID

FIGURE C-2. St. Louis RAPS grid.

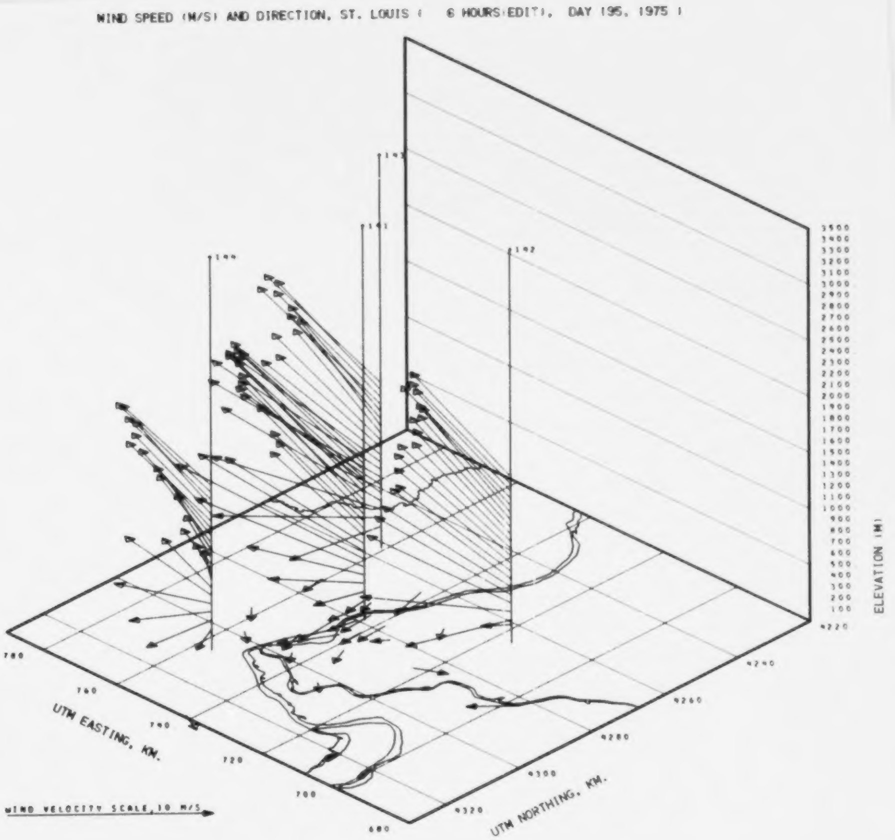


FIGURE C-3. Three-dimensional plot showing variation of horizontal wind speed and direction for both surface and upper air.

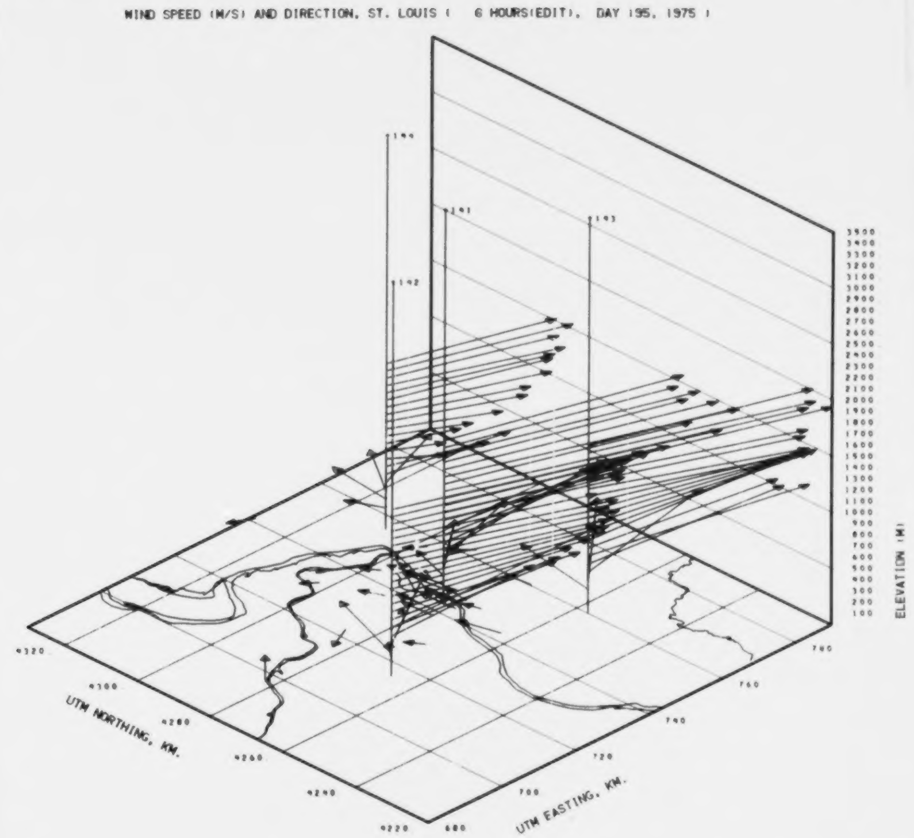


FIGURE C-4. Three-dimensional plot like Fig. C-3 but rotated 90° clockwise in the X,Y plane.

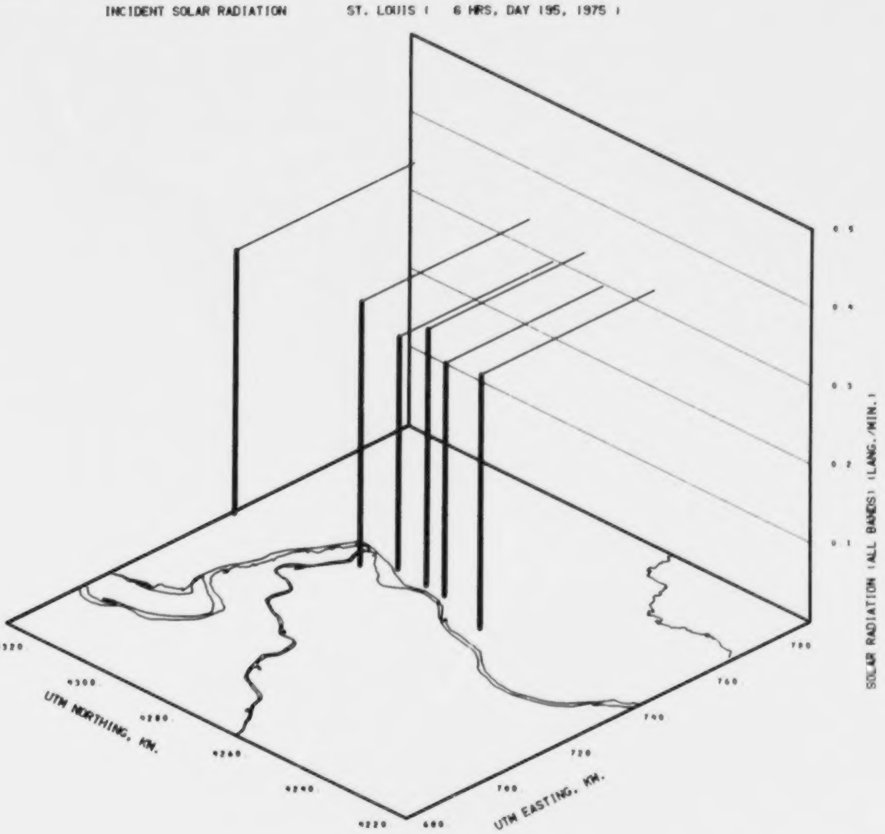


FIGURE C-5. Three-dimensional plot showing total incident solar radiation.

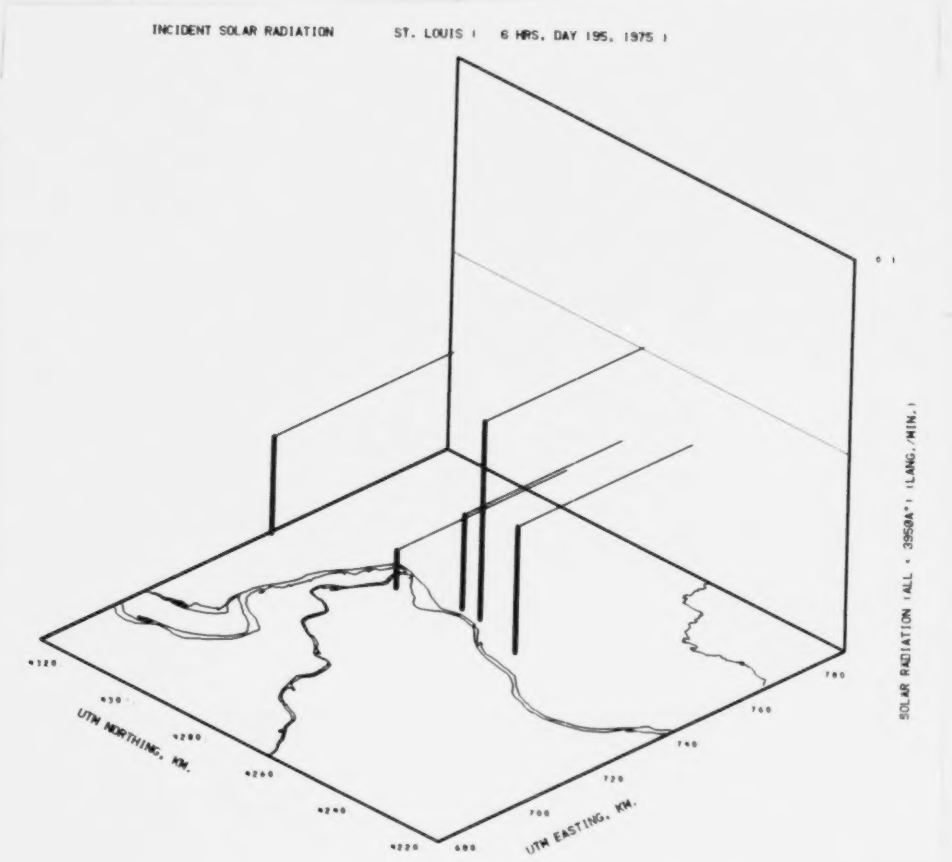


FIGURE C-6. Three-dimensional plot like Fig. C-5 but showing only wavelengths <3950 Å.

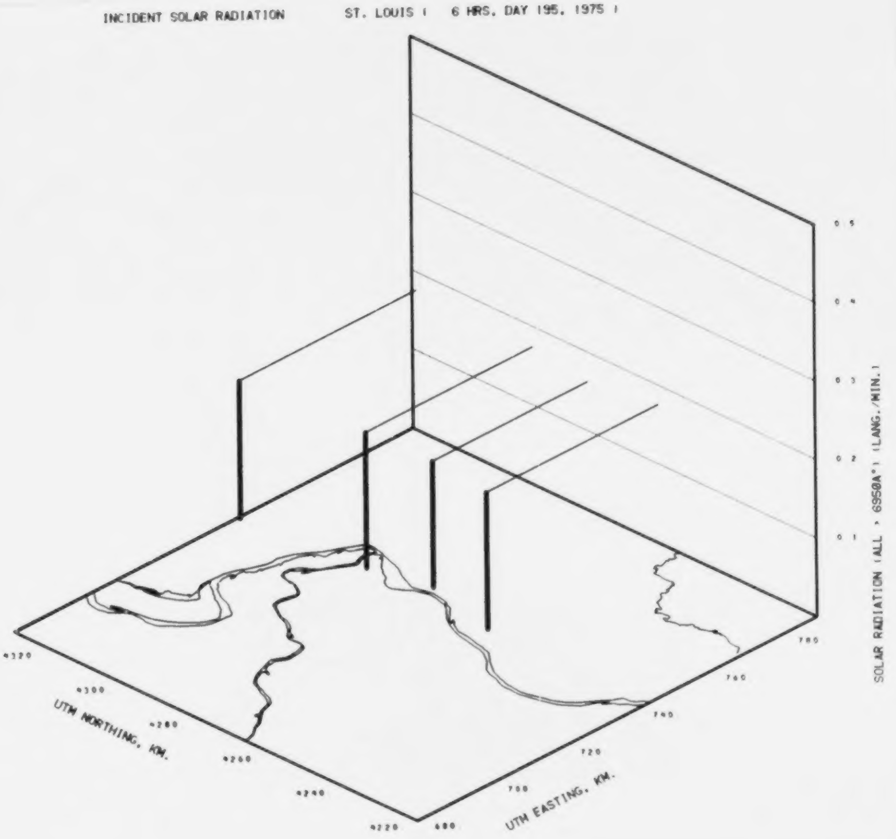


FIGURE C-7. Three-dimensional plot like Fig. C-5 but showing only wavelengths >6950 Å.

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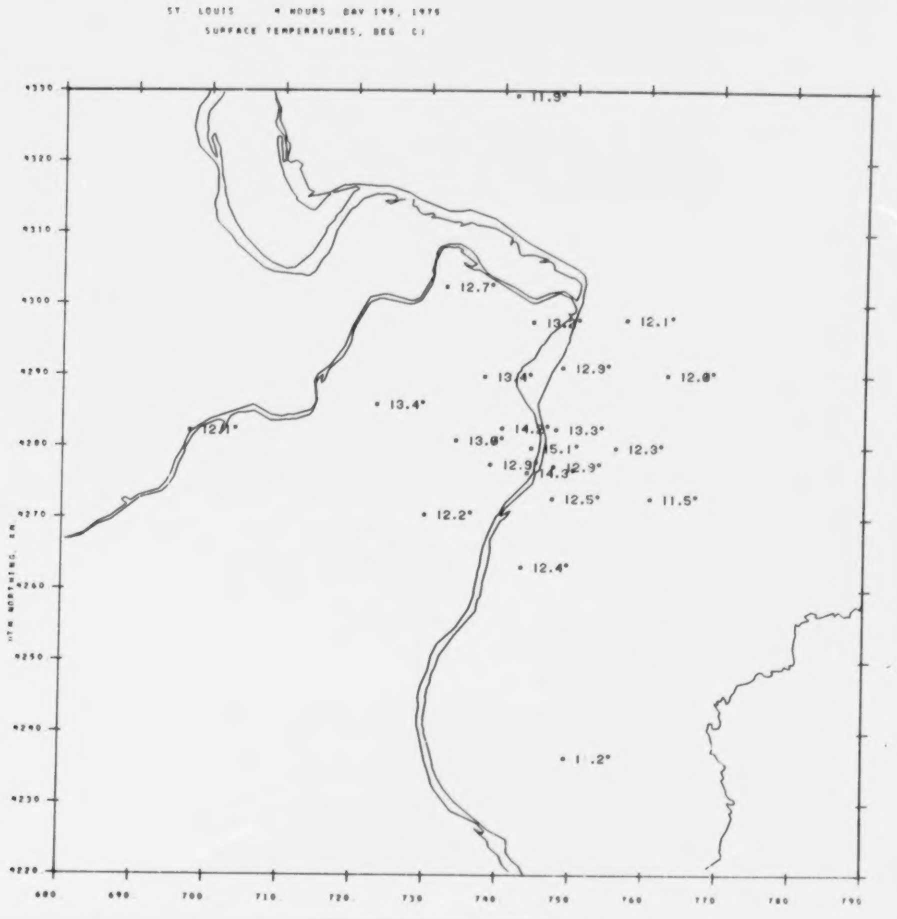
ST. LOUIS 4 HOURS DAY 199, 1975
SURFACE TEMPERATURES, DEG C)
UTM NORTHING, KM
4330
4320
4310
4300
4290
4280
4270
4260
4250
4240
4230
4220
680
690
700
710
720
730
740
750
760
770
780
790
11.9°
12.7°
13.2°
12.1°
13.4°
12.9°
12.8°
13.4°
12.1°
14.2°
13.3°
13.8°
15.1°
12.3°
12.9°
12.9°
14.3°
12.5°
11.5°
12.2°
12.4°
11.2°

FIGURE C-8. Two-dimensional, horizontal plot of surface temperature.

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PAGE NUMBER

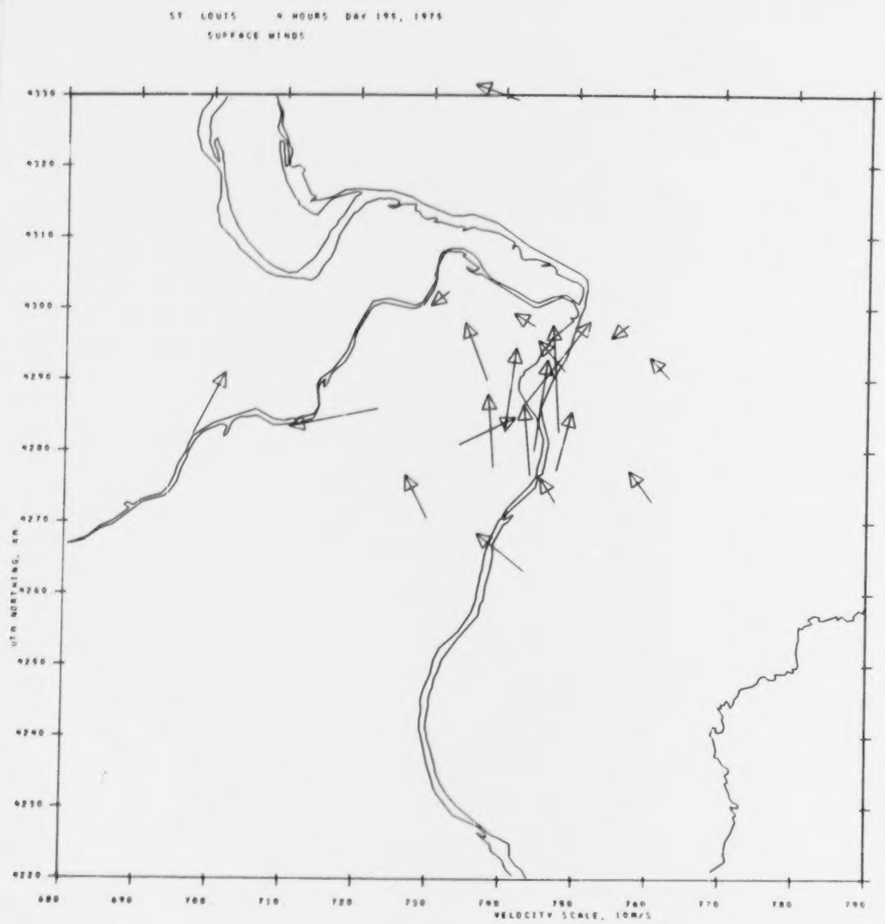
ST. LOUIS 9 HOURS DAY 195, 1975
SURFACE WINDS
4330
4320
4310
4300
4290
4280
4270
4260
4250
4240
4230
4220
UTM NORTHING, KM
680
690
700
710
720
730
740
750
760
770
780
790
VELOCITY SCALE, 10M/S

FIGURE C-9. Two-dimensional, horizontal plot of surface winds.

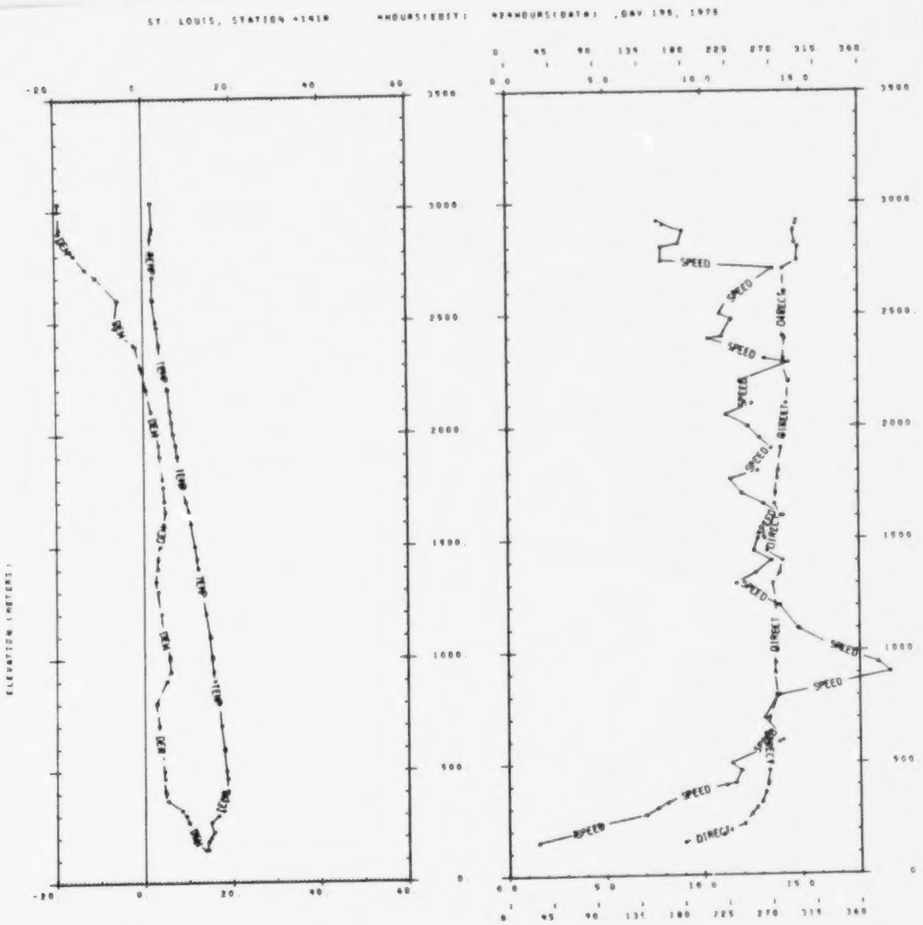

FIGURE C-10. Vertical scalar plot of upper air station data, including temperature, dew point, wind speed, and wind direction.

APPENDIX D

Q-PROCESSOR

DESCRIPTION

The Q-Processor (QPROC) is written in PASCAL, a block-structured language with many useful control and data structures. The record structure in the language implements the data base of the code. A record structure is an array of records; each record contains several data fields. These fields are not necessarily the same for all records in a given structure. The data structures are, thus, flexible and comprehensive.

After initialization procedures, QPROC reads all the editing instructions from the user-generated file INPUT into a record structure called CHANGE. The fields of each record in CHANGE correspond to the fields of an editing instruction. Depending on the option field of the instruction, the location field may contain the station number, or it may have two subfields containing a coordinate pair, or it may not exist. After this mixing height data for the day is read from data file MIXHGT.

The rest of the processing is done an hour at a time. Each hour, meteorological data from data file RAMSDAT is stored within the code in a record structure called RMSDAT. For every station, this structure contains a record consisting of fields for station specification (UTM coordinates or station number), station name if one exists, and each of the items required for the output QPMET file. One variable is examined at a time and those that are not required for the analysis being performed are skipped completely. Surface wind speed and direction are read directly from the file RAMSDAT to the RMSDAT record structure. Pyranometer data are divided by the computed average solar flux (Luther and Gelinas, 1975; MacCracken and Sauter, 1975) for the hour to generate optical transmissivities. Mean wind speeds and directions are entered via editing commands. Changes in the inversion height values read from MIXHGT are also made via the editing commands.

As the variables in the RAMSDAT file are being scanned, pollutant concentrations are read into QPROC and written to the QICON file in the appropriate format. All hydrocarbon and methane data in RAMSDAT are used to compute values for the hydrocarbon species required by LIRAQ, i.e., HC1 (alkenes), HC2 (alkanes), HC4 (aldehydes), according to the formula:

HC1 = maximum of (total hydrocarbon-methane or 0.01) * 0.20 * 0.10

HC2 = maximum of (total hydrocarbon-methane or 0.01) * 0.20 * 0.87

HC4 = maximum of (total hydrocarbon-methane or 0.01) * 0.20 * 0.03 .

After the hourly record in RAMSDAT has been scanned, each of the editing instructions is processed. If the current hour is within the time limits of an instruction, the specified alteration is made in the RMSDAT data structure. After all the instructions have been processed, the data in RMSDAT are sent to the QPMET file in the format required by the M-Processor.

Flowcharts of the QPROC main routine, procedure READCHNG, procedure READHOUR, and procedure READDATA appear in Figs. D-1 through D-4, respectively.

INPUT FILES

RAMSDAT

This file contains EPA meteorological data for a one-day period. The first section of RAMSDAT may contain upper air data, which QPROC does not examine. An 89 in the first two columns of an input line causes this part of the file to terminate. Following any upper air data is an hour-by-hour list of surface data from the 25 St. Louis stations. An hourly data set comprises 22 variable records. Each variable record consists of a lead card followed by 25 numbers. The lead card contains the variable indicator along with the hour, day, and year in (I2, I5, I4, I5) format. The variable indicators appear in Table D-1. This file is identical to the RAMS file discussed in Appendix C. See Fig. D-5 for a sample of an hourly record from input file RAMSDAT.

INPUT

The first line of this file contains the latitude, local noon (in seconds) of the region of interest, the Julian day, and year of the data is blank delimited real numbers. Editing instructions constitute the remainder of the file. These editing instructions give the user the capability of specifying one or more, possibly overlapping, changes to the St. Louis meteorological data. Overlapping changes are processed in the order specified. Each instruction has the following blank delimited fields: OPTION, ITEM, CONSTANT, STARTTIME, STOPTIME, LOCATION.

The OPTION field determines the type of change to be made. Valid options are summarized in Table D-2.

The ITEM field determines the data item to be changed by this instruction. Valid data items are:

- SSF - surface wind speed.
- DSF - surface wind direction.
- SMN - mean wind speed.
- DMN - mean wind direction.
- IHT - inversion height.
- OPT - optical transmissivity.

The CONSTANT field consists of a single floating-point constant that will be applied to the ITEM field in a manner determined by the OPTION field.

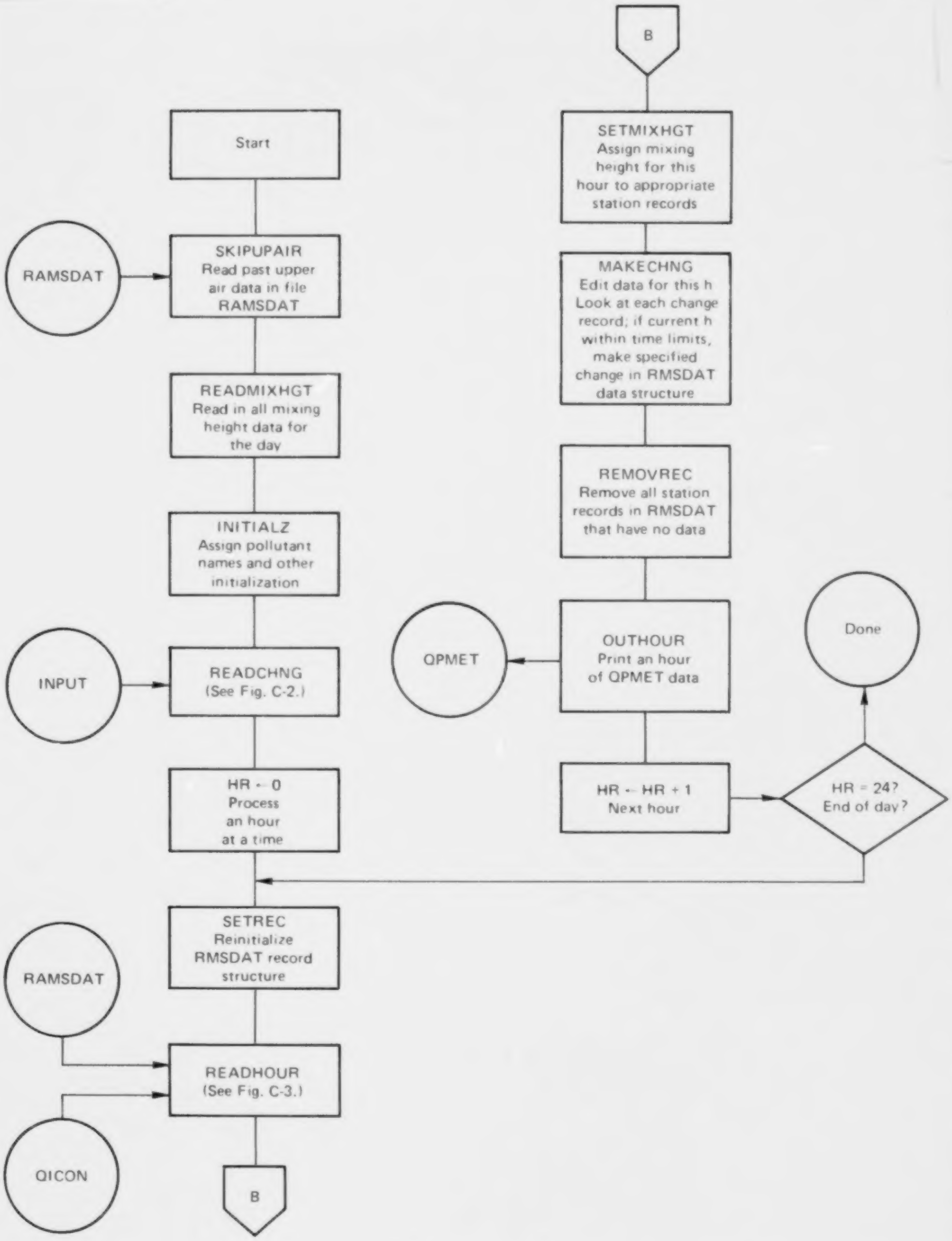
B
Start
SETMIXHGT
Assign mixing height for this hour to appropriate station records
RAMSDAT
SKIPUPAIR
Read past upper air data in file RAMSDAT
MAKECHNG
Edit data for this h
Look at each change record; if current h within time limits, make specified change in RMSDAT data structure
READMIXHGT
Read in all mixing height data for the day
REMOVREC
Remove all station records in RMSDAT that have no data
INITIALZ
Assign pollutant names and other initialization
Done
QPMET
OUTHOUR
Print an hour of QPMET data
INPUT
READCHNG
(See Fig. C-2.)
HR ← 0
Process an hour at a time
HR ← HR + 1
Next hour
HR = 24?
End of day?
SETREC
Reinitialize RMSDAT record structure
RAMSDAT
READHOUR
(See Fig. C-3.)
QICON
B

FIGURE D-1. **Q-Processor flowchart, main routine. Procedure (subroutine) calls are indicated by a capitalized procedure name in a process box.**

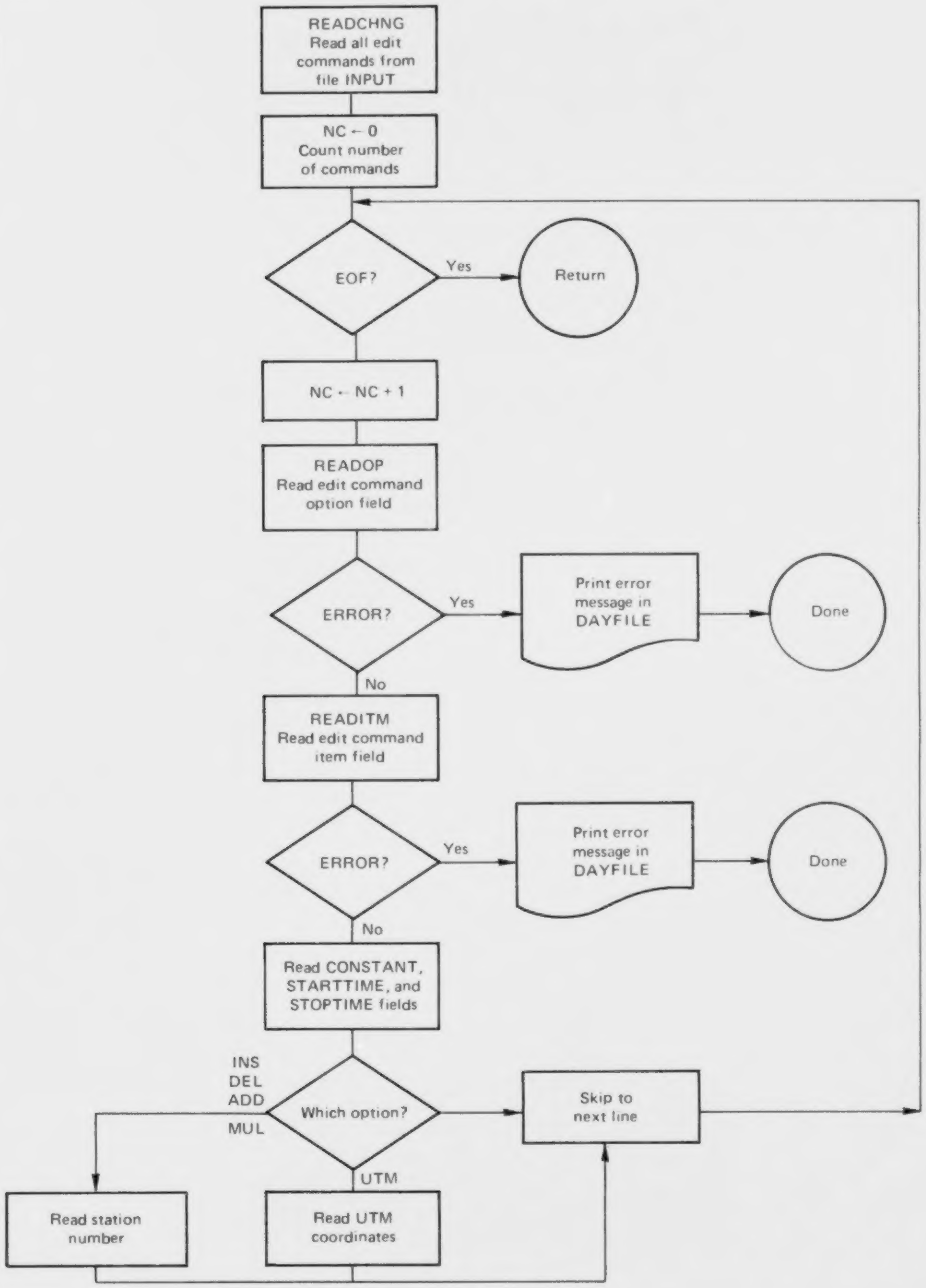
READCHNG
Read all edit commands from file INPUT
NC ← 0
Count number of commands
EOF?
Yes
Return
NC ← NC + 1
READOP
Read edit command option field
ERROR?
Yes
Print error message in DAYFILE
Done
No
READITM
Read edit command item field
ERROR?
Yes
Print error message in DAYFILE
Done
No
Read CONSTANT, STARTTIME, and STOPTIME fields
INS
DEL
ADD
MUL
Which option?
UTM
Skip to next line
Read station number
Read UTM coordinates

FIGURE D-2. Q-Processor flowchart, procedure READCHGN.

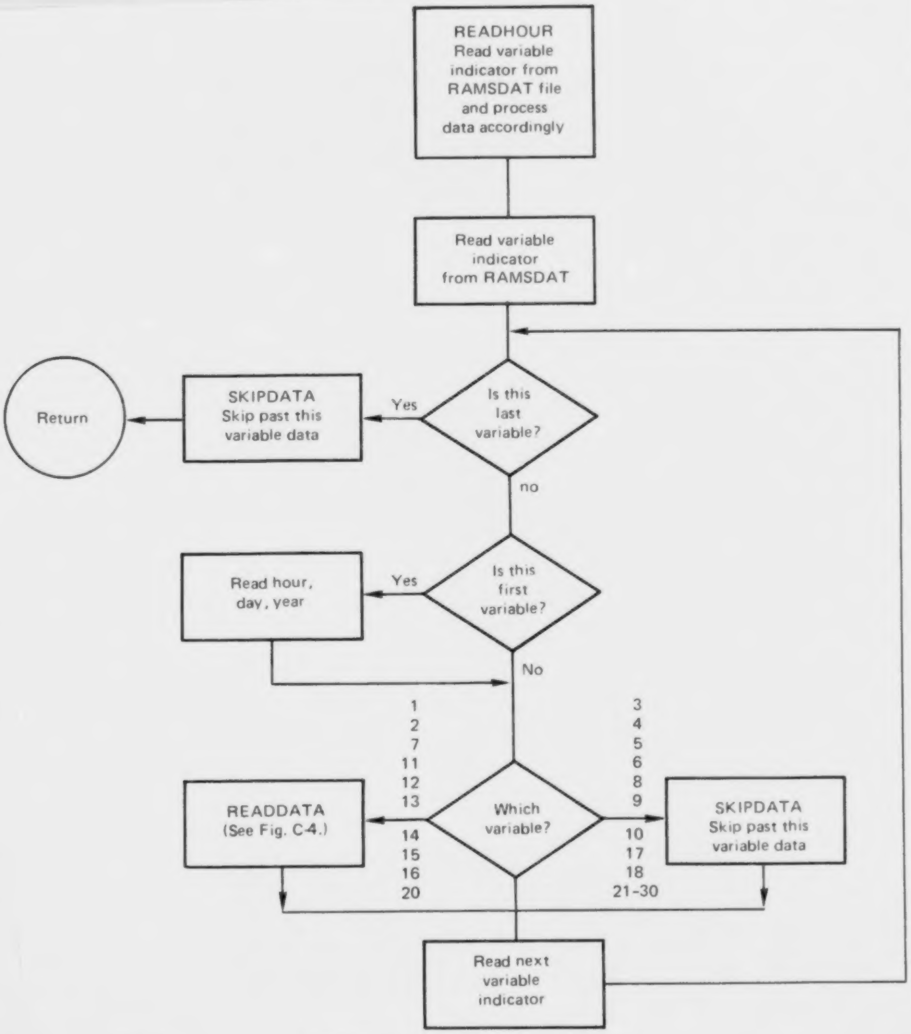
READHOUR
Read variable indicator from RAMSDAT file and process data accordingly
Read variable indicator from RAMSDAT
Is this last variable?
Yes
SKIPDATA
Skip past this variable data
Return
no
Is this first variable?
Yes
Read hour, day, year
No
1
2
7
11
12
13
14
15
16
20
3
4
5
6
8
9
10
17
18
21-30
Which variable?
READDATA
(See Fig. C-4.)
SKIPDATA
Skip past this variable data
Read next variable indicator

FIGURE D-3. Q-Processor flowchart, procedure READHOUR.

STARTTIME and STOPTIME specify the time limits during which a change will be made. Changes will be made from STARTTIME through and including the hour beginning with STOPTIME. These fields are both integers from 0 to 23.

The LOCATION field consists of either a station number or a UTM easting-northing coordinate pair, or it may be empty, depending on the option selected. A station number is an integer between 1 and 25 for surface stations or an integer between 41 and 45 for upper air stations. UTM coordinates are real numbers.

INS, ADD, MUL, and DEL require a station number in the LOCATION field. UTM requires a UTM coordinate pair in that field, whereas with RID and CPY the field should be blank. See Fig. D-6 for an example of a Q-Processor INPUT file.

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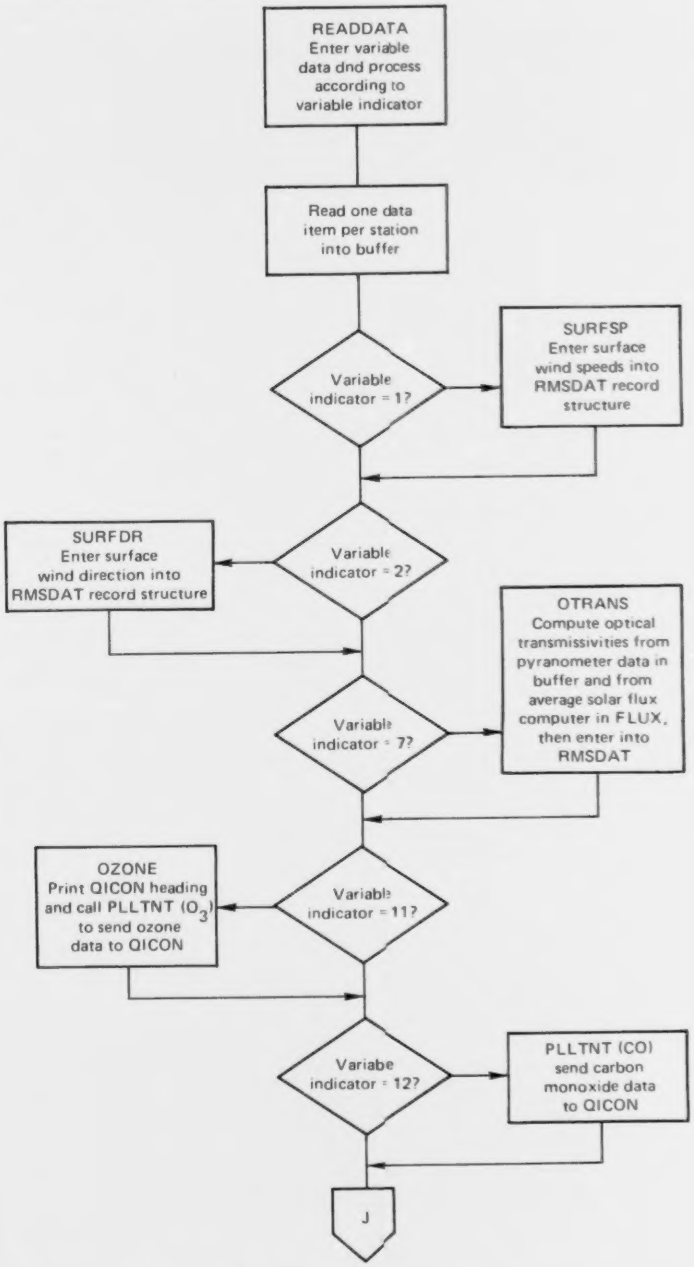
READDATA
Enter variable data dnd process according to variable indicator
Read one data item per station into buffer
Variable indicator = 1?
SURFSP
Enter surface wind speeds into RMSDAT record structure
Variable indicator = 2?
SURFDR
Enter surface wind direction into RMSDAT record structure
OTRANS
Compute optical transmissivities from pyranometer data in buffer and from average solar flux computer in FLUX, then enter into RMSDAT
Variable indicator = 7?
OZONE
Print QICON heading and call PLLTNT (O3) to send ozone data to QICON
Variable indicator = 11?
Variabe indicator = 12?
PLLTNT (CO)
send carbon monoxide data to QICON
J

FIGURE D-4. Q-Processor flowchart, procedure READDATA.

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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

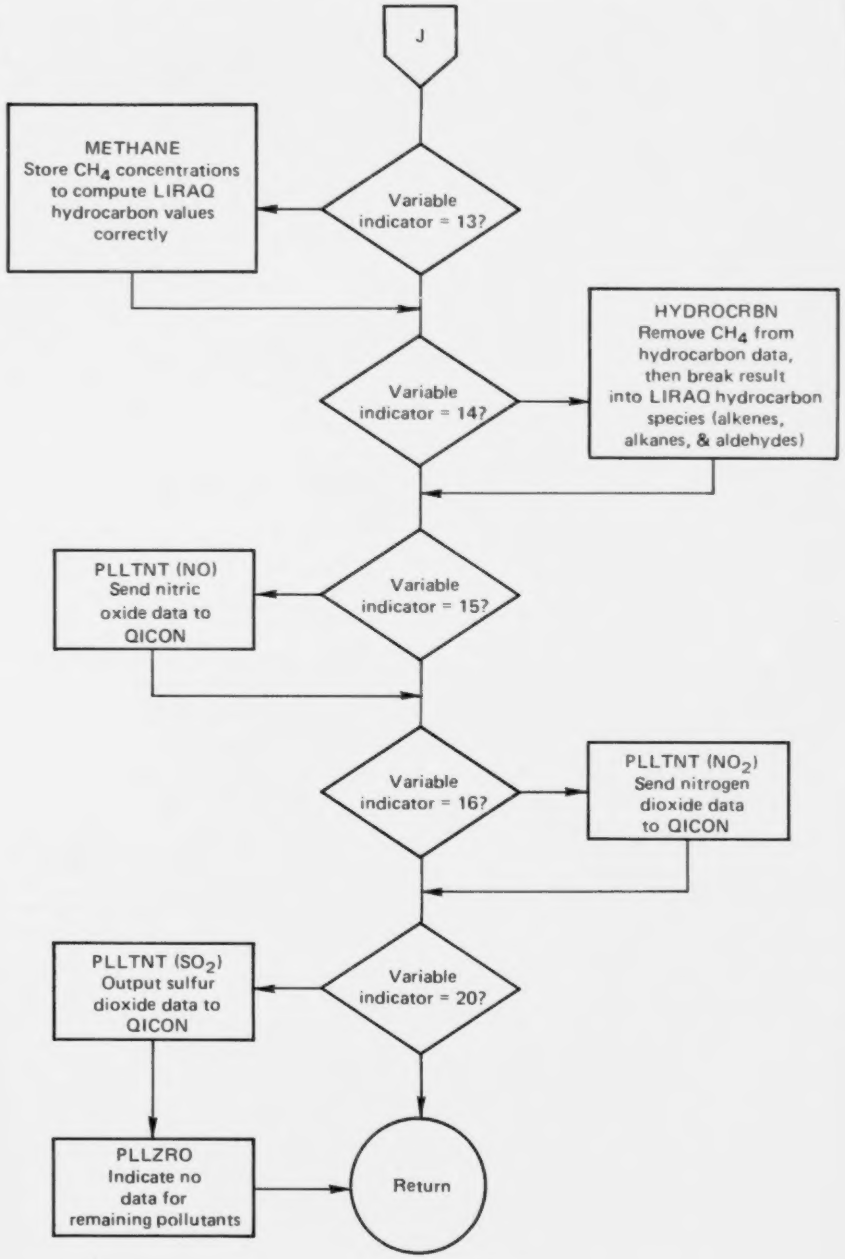
J
METHANE
Store CH4 concentrations to compute LIRAQ hydrocarbon values correctly
Variable indicator = 13?
HYDROCRBN
Remove CH4 from hydrocarbon data, then break result into LIRAQ hydrocarbon species (alkenes, alkanes, & aldehydes)
Variable indicator = 14?
PLLTNT (NO)
Send nitric oxide data to QICON
Variable indicator = 15?
Variable indicator = 16?
PLLTNT (NO2)
Send nitrogen dioxide data to QICON
PLLTNT (SO2)
Output sulfur dioxide data to QICON
Variable indicator = 20?
PLLZRO
Indicate no data for remaining pollutants
Return

FIGURE D-4. Continued.

TABLE D-1. Variable indicators for lead cards containing surface data in the RAMS file.

Variable	Indicator	Units
Wind speed	WS	m/s
Wind direction	WD	deg clockwise from north
Temperature	T	°C
Dew point	DP	°C
Barometric pressure	BP	mbar
Temperature difference	DT	°C (difference between 30-m level and 6-m level)
Pyranometer	PYRA(1)	Langleys/min, all wave lengths
Pyranometer	PYRA(2)	Langleys/min, greater than 3950 Å
Pyranometer	PYRA(3)	Langleys/min, greater than 6950 Å
Pyrgeometer	PYRG	Langleys/min
Ozone	O_3	ppm by vol
Carbon monoxide	CO	ppm by vol
Methane	CH_4	ppm by vol
Total hydrocarbons	THC	ppm by vol (carbon)
Nitric oxide	NO	ppm by vol
Nitrogen dioxide	NO_2	ppm by vol
Oxides of nitrogen	NO_x	ppm by vol
Total particulate sulfur	TS	ppm by vol
Hydrogen sulfide	H_2S	ppm by vol
Sulfur dioxide	SO_2	ppm by vol
Nephelometer	NEPH(1)	m^{-1}
Nephelometer	NEPH(2)	m^{-1}

```
  18  500 181 1976        .72576-01    .49326-01    .11113-01    .25000-02    .25884-02

                          .10000+38    .34932-01    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .25000-02    .25000-02    .98170-02
                          .51703-01    .82690-02    .10000+38    .10000+38    .10000+38
                          .10000+38    .25000-02    .25000-02    .45074-02    .10000+38
  19  500 181 1976        .10000+38    .10000+38    .25000-02    .25000-02    .25000-02

                          .25000-02    .10000+38    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .25000-02    .10000+38    .10000+38
                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
  20  500 181 1976        .10000+38    .10000+38    .10000+38    .10000+38    .10000+38

                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .25000-02    .10000+38    .10000+38
                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
  21  500 181 1976        .10000+38    .10000+38    .10000+38    .10000+38    .10000+38

                          .85449-04    .14642-03    .67397-04    .61892-04    .77158-04
                          .61609-04    .68433-04    .22018-03    .14941-04    .54158-04
                          .17487-03    .82387-04    .98506-04    .18373-03    .16563-04
                          .21135-04    .46649-04    .63796-04    .91785-05    .10000+38
  22  500 181 1976        .25921-04    .41614-04    .82965-04    .34234-04    .26616-04

                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
   1  600 181 1976        .10000+38    .10000+38    .10000+38    .10000+38    .10000+38

                          .29703+01    .26205+01    .27216+01    .10000+38    .32586+01
                          .25552+01    .24348+01    .26395+01    .20968+01    .20623+01
                          .25674+01    .22157+01    .24662+01    .24256+01    .22834+01
                          .17853+01    .22531+01    .15763+01    .20950+01    .16887+01
   2  600 181 1976        .21576+01    .39155+01    .27369+01    .63251+01    .14349+01

                          .21683+03    .22249+03    .22000+03    .10000+38    .21011+03
                          .21357+03    .22044+03    .21658+03    .21167+03    .22656+03
                          .20865+03    .20343+03    .20249+03    .20858+03    .19110+03
                          .18428+03    .21394+03    .21016+03    .19955+03    .18835+03
   3  600 181 1976        .20909+03    .18785+03    .18138+03    .20299+03    .20763+03

                          .23259+02    .23235+02    .22424+02    .22272+02    .23088+02
                          .22415+02    .23232+02    .22357+02    .21985+02    .21893+02
                          .21999+02    .22234+02    .22036+02    .22254+02    .21836+02
                          .21555+02    .21642+02    .20943+02    .21645+02    .21463+02
   4  600 181 1976        .22324+02    .20507+02    .21601+02    .22250+02    .20813+02

                          .16974+02    .19883+02    .10000+38    .10000+38    .23672+02
                          .19813+02    .10000+38    .19768+02    .87894+01    .81938+01
                          .20268+02    .23214+02    .10000+38    .19106+02    .10000+38
                          .18704+02    .90566+01    .10000+38    .14113+02    .10000+38
   5  600 181 1976        .21543+02    .19421+02    .10000+38    .15653+02    .10000+38

                          .29394+02    .10000+38    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .10000+38    .29467+02    .10000+38
                          .10000+38    .29327+02    .10000+38    .10000+38    .10000+38
                          .10000+38    .10000+38    .10000+38    .10000+38    .10000+38
   6  600 181 1976        .10000+38    .29231+02    .29358+02    .29170+02    .29377+02
```

FIGURE D-5. Example of an hourly record from input file RAMSDAT.

MIXHGT

Mixing height (inversion height) data for several days are contained in the file MIXHGT. Data for one day consist of a lead card followed by four station records. The lead card contains the day and year in (2I5) format. Each station record requires two cards, the first card with data for hours 0 to 11, the second card with data hours 12 to 23. Each card is in (13X,12I5) format. The four station records give the mixing height values for each of the upper air stations (numbered 41 to 44) in order. See Fig. D-7 for an example of several daily records from MIXHGT.

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TABLE D-2. List of valid options and their meanings.

Options	Meaning
INS	Specify the value of ITEM at a station to be the value of CONSTANT. This overwrites any previous value of this item at the station within the specified time constraints.
ADD	Add CONSTANT to the present value of ITEM at a station. This option should not be used to change item fields which have been flagged as missing data.
MUL	Multiply the current value of ITEM by CONSTANT at a station. This option should not be used to change item fields which have been previously flagged as missing data.
DEL	Delete ITEM at a station. The specified item field is flagged as missing data. If all item fields for a station are missing data, the station will be eliminated from the output for the current hour. The CONSTANT field must contain some numeric value although this field is not used.
UTM	Specify the value of ITEM at a UTM location to be the value of CONSTANT. If a UTM station at the coordinates has not previously been defined, a new record is created with the value of ITEM set to CONSTANT and the location defined by UTM coordinates. This allows bogus data to be added at any point in the region of interest.
RID	Delete the specified ITEM field from all surface stations (1-25) within the specified time constraints.
CPY	Specify the value of ITEM for all surface stations (1-25) within the specified time constraints.

OUTPUT FILE

QPMET

This file consists of hourly data sets containing meteorological data specified by station and/or by UTM easting-northing coordinate pairs. Each logical station record within a data set specifies for a single station the station symbol, the station number, surface wind speed, surface wind direction, mean wind speed, mean wind direction, inversion base height, and optical transmissivity of the atmosphere. Fields for which no data exist are filled with the missing data flag "-9999." The end of the station subset of an hourly data set is flagged by a record having a negative or zero station number.

The format of a UTM subset of an hourly data set is nearly identical to that of a station subset. Within a logical UTM record, the station symbol and station number fields have been replaced with a UTM easting field and a UTM northing field. The UTM subset is ended by a logical record with a negative or zero easting.

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EPA-287 (Cin.)
(4-76)

```
  38.63 43260.
 INS SMN    6.2   9  9  20
 INS DMN  274.    9  9  20
 INS SMN    7.05 10 10   4
 INS DMN  251.   10 10   4
 DEL SSF    0     9  9   4
 CPY IHT  850.    9 10
 RID DSF    0     9  9
 ADD OPT   10.    9 10  22
 UTM SMN    6.5  10 10  654.9  4215.25
 UTM DMN  301.   10 10  654.9  4215.25
 UTM DSF  256.    9 10  701 4012.
UTM SSF   7.1    10 10   701. 4012.0
 MUL SSF  100.    9 10   1
 UTM IHT 1050.    9 10 654.9         4215.25
      DEL  OPT      0           9 9
 DEL IHT    0     9  9   4
```

An explanation of editing instructions contained in this file is listed below according to the line in which they appear.

Line

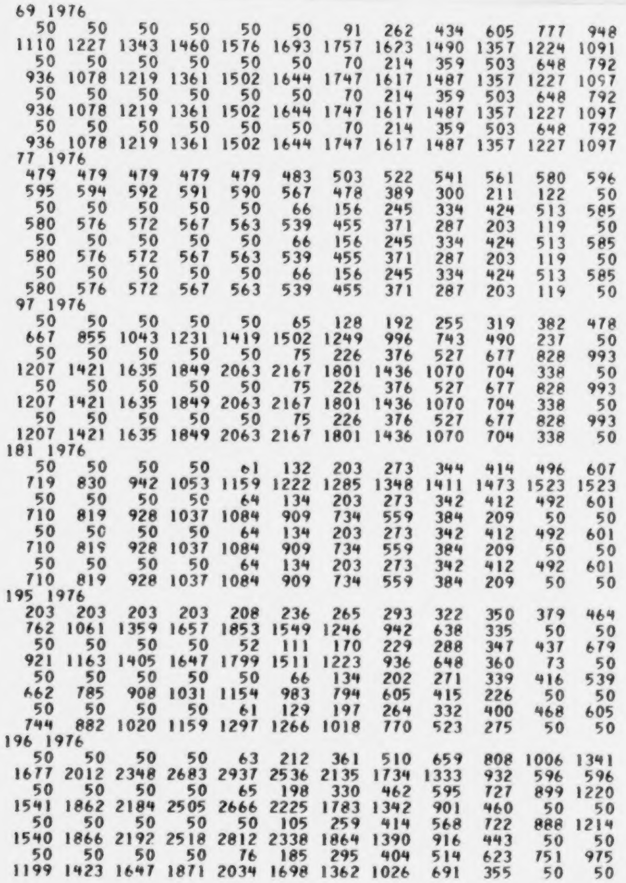
1. Latitude, local noon
2. Insert a mean wind speed of 6.2 m/s at station 20 for hour 9
3. Insert a mean wind direction of 274° at station 2 for hour 9
4. Insert a mean wind speed of 7.05 m/s at station 4 for hour 10
5. Insert a mean wind direction of 251° at station 4 for hour 10
6. Delete surface wind speed from station 4 for hour 9
7. Set inversion height of 850 m at all stations for hours 9 and 10
8. Delete surface wind directions from all stations for hour 9
9. Add 10. Langleys to the optical transmissivity at station 22 for hours 9 and 10
10. Insert a mean wind speed at UTM coordinates 654.9 east and 4215.25 north for hour 10
11. Insert a mean wind direction at the same UTM position as line 10 for hour 10
12. Insert a surface wind direction at UTM coordinates 701. east and 4012. north for hours 9 and 10
13. Insert a surface wind speed at the same UTM coordinates as line 12 for hour 10
14. Multiply surface wind speed by 100. at station 1 for hours 9 and 10
15. Insert inversion height of 1050. m at the same UTM coordinates as line 10 for hours 9 and 10
16. Delete optical transmissivity from station 4 for hour 9
17. Delete inversion height from station 4 for hour 9

Fields are blank delimited and may be anywhere on a line. Line numbers shown above are not part of the file. The instructions would normally be left justified in a line.

FIGURE D-6. Example of a Q-Processor INPUT file.

Note that a data set must be present for each hour, even if both of its subsets are empty. The QPMET file format is shown in Table D-3.

See Fig. D-8 for an example of two hourly records from a QPMET file where the data from the RAMSDAT file has not been edited (a) and where the data has been changed (b) according to the editing instructions shown in Fig. D-6.



```
 69 1976
   50   50   50   50   50   50   91  262  434  605  777  948
 1110 1227 1343 1460 1576 1693 1757 1623 1490 1357 1224 1091
   50   50   50   50   50   50   70  214  359  503  648  792
  936 1078 1219 1361 1502 1644 1747 1617 1487 1357 1227 1097
   50   50   50   50   50   50   70  214  359  503  648  792
  936 1078 1219 1361 1502 1644 1747 1617 1487 1357 1227 1097
   50   50   50   50   50   50   70  214  359  503  648  792
  936 1078 1219 1361 1502 1644 1747 1617 1487 1357 1227 1097
 77 1976
  479  479  479  479  479  483  503  522  541  561  580  596
  595  594  592  591  590  567  478  389  300  211  122   50
   50   50   50   50   50   66  156  245  334  424  513  585
  580  576  572  567  563  539  455  371  287  203  119   50
   50   50   50   50   50   66  156  245  334  424  513  585
  580  576  572  567  563  539  455  371  287  203  119   50
   50   50   50   50   50   66  156  245  334  424  513  585
  580  576  572  567  563  539  455  371  287  203  119   50
 97 1976
   50   50   50   50   50   65  128  192  255  319  382  478
  667  855 1043 1231 1419 1502 1249  996  743  490  237   50
   50   50   50   50   50   75  226  376  527  677  828  993
 1207 1421 1635 1849 2063 2167 1801 1436 1070  704  338   50
   50   50   50   50   50   75  226  376  527  677  828  993
 1207 1421 1635 1849 2063 2167 1801 1436 1070  704  338   50
   50   50   50   50   50   75  226  376  527  677  828  993
 1207 1421 1635 1849 2063 2167 1801 1436 1070  704  338   50
181 1976
   50   50   50   50   61  132  203  273  344  414  496  607
  719  830  942 1053 1159 1222 1285 1348 1411 1473 1523 1523
   50   50   50   50   64  134  203  273  342  412  492  601
  710  819  928 1037 1084  909  734  559  384  209   50   50
   50   50   50   50   64  134  203  273  342  412  492  601
  710  819  928 1037 1084  909  734  559  384  209   50   50
   50   50   50   50   64  134  203  273  342  412  492  601
  710  819  928 1037 1084  909  734  559  384  209   50   50
195 1976
  203  203  203  203  208  236  265  293  322  350  379  464
  762 1061 1359 1657 1853 1549 1246  942  638  335   50   50
   50   50   50   50   52  111  170  229  288  347  437  679
  921 1163 1405 1647 1799 1511 1223  936  648  360   73   50
   50   50   50   50   50   66  134  202  271  339  416  539
  662  785  908 1031 1154  983  794  605  415  226   50   50
   50   50   50   50   61  129  197  264  332  400  468  605
  744  882 1020 1159 1297 1266 1018  770  523  275   50   50
196 1976
   50   50   50   50   63  212  361  510  659  808 1006 1341
 1677 2012 2348 2683 2937 2536 2135 1734 1333  932  596  596
   50   50   50   50   65  198  330  462  595  727  899 1220
 1541 1862 2184 2505 2666 2225 1783 1342  901  460   50   50
   50   50   50   50   50  105  259  414  568  722  888 1214
 1540 1866 2192 2518 2812 2338 1864 1390  916  443   50   50
   50   50   50   50   76  185  295  404  514  623  751  975
 1199 1423 1647 1871 2034 1698 1362 1026  691  355   50   50
```

FIGURE D-7. Example of several daily records from file MIXHGT.

QICON

This file is composed of 24 hourly data sets containing pollutant concentration data specified by station. The file format provides for specification by UTM coordinates, but the Q-Processor does not use this feature. The hourly data are composed of a data set for each pollutant. These data include a station-by-station list of the concentration of the particular pollutant. Stations with missing data are not listed. Values for alkenes, alkanes, and aldehydes are computed as fractions of the reported total hydrocarbon concentration minus the methane concentration. A pollutant data set must be present for each pollutant in LIRAQ, even if the data set is empty. The QICON file format is shown in Table D-4. See Fig. D-9 for samples of QICON header cards and an hourly record.

TABLE D-3. Format for QPMET file.

Card Format	Information
(A4,1X,I2,1X,I3,1X,I4)	Start of time-set card, containing the literal-timeset-followed by hour, date of year, and year.
(5X,A1,6X,I4,4F10.2,F10.1,F10.3)	Station symbol, station number, surface wind speed, surface wind direction, mean wind speed, mean wind direction, inversion-base height, and optical transmissivity. Wind speeds are in m/s; inversion base height, in m above mean sea level. The station subset of the time set is terminated by a record with a negative or zero station number.
(2X,F7.3,7X,F2.3,4F10.2,F10.1,F10.3)	UTM easting and northing, surface wind speed, surface wind direction, mean wind speed, mean wind direction, inversion-base height, and optical transmissivity. Wind speeds are in m/s; inversion-base height, in m above mean sea level. The UTM subset of the time set is terminated by a record with a negative or zero UTM easting.

```
*TIMESET  9 191 1975
    +101          1      4.75    291.44  -9999.00  -9999.00    -9999.0 -9999.000
    +103          3  -9999.00    316.08  -9999.00  -9999.00    -9999.0     0.657
    +104          4      4.70    318.46  -9999.00  -9999.00    -9999.0     0.562
    +105          5      4.78    299.57  -9999.00  -9999.00    -9999.0 -9999.000
    +106          6      5.21    300.81  -9999.00  -9999.00    -9999.0 -9999.000
    +107          7      4.11    297.36  -9999.00  -9999.00    -9999.0 -9999.000
    +108          8      4.25    302.31  -9999.00  -9999.00    -9999.0     0.640
    +109          9      5.36    318.55  -9999.00  -9999.00    -9999.0 -9999.000
    +110         10      4.13    278.92  -9999.00  -9999.00    -9999.0 -9999.000
    +112         12      4.61  -9999.00  -9999.00  -9999.00    -9999.0 -9999.000
    +113         13      4.51    288.12  -9999.00  -9999.00    -9999.0 -9999.000
    +114         14      3.96    293.89  -9999.00  -9999.00    -9999.0     0.471
    +115         15      3.96    276.41  -9999.00  -9999.00    -9999.0 -9999.000
    +116         16      4.09    317.91  -9999.00  -9999.00    -9999.0 -9999.000
    +117         17      3.78    289.79  -9999.00  -9999.00    -9999.0 -9999.000
    +118         18      3.23    285.90  -9999.00  -9999.00    -9999.0     0.661
    +119         19      3.98    283.38  -9999.00  -9999.00    -9999.0 -9999.000
    +120         20      4.63  -9999.00  -9999.00  -9999.00    -9999.0 -9999.000
    +121         21      3.18    294.24  -9999.00  -9999.00    -9999.0 -9999.000
    +122         22      4.36  -9999.00  -9999.00  -9999.00    -9999.0     0.841
    +123         23      4.95    305.40  -9999.00  -9999.00    -9999.0 -9999.000
    +125         25      4.81    287.35  -9999.00  -9999.00    -9999.0 -9999.000
                  0     0         0         0         0           0      0
  0         0           0         0         0         0           0      0
*TIMESET 10 191 1975
    +101          1      4.67    287.70  -9999.00  -9999.00    -9999.0 -9999.000
    +102          2  -9999.00    320.77  -9999.00  -9999.00    -9999.0 -9999.000
    +103          3      6.41    309.22  -9999.00  -9999.00    -9999.0     0.790
    +104          4      4.19    303.94  -9999.00  -9999.00    -9999.0     0.605
    +105          5      5.63    293.14  -9999.00  -9999.00    -9999.0 -9999.000
    +106          6      5.65    303.79  -9999.00  -9999.00    -9999.0 -9999.000
    +107          7      4.97    297.17  -9999.00  -9999.00    -9999.0 -9999.000
    +108          8      5.25    298.36  -9999.00  -9999.00    -9999.0     0.880
    +109          9      5.12  -9999.00  -9999.00  -9999.00    -9999.0 -9999.000
    +110         10      4.51    289.02  -9999.00  -9999.00    -9999.0 -9999.000
    +112         12      4.86  -9999.00  -9999.00  -9999.00    -9999.0 -9999.000
    +113         13      5.82    279.59  -9999.00  -9999.00    -9999.0 -9999.000
    +114         14      4.31    302.25  -9999.00  -9999.00    -9999.0     0.901
    +115         15      4.68    290.54  -9999.00  -9999.00    -9999.0 -9999.000
    +116         16      4.18    307.65  -9999.00  -9999.00    -9999.0 -9999.000
    +117         17      4.00    319.63  -9999.00  -9999.00    -9999.0 -9999.000
    +118         18      3.28    292.76  -9999.00  -9999.00    -9999.0     0.578
    +119         19      4.06    286.57  -9999.00  -9999.00    -9999.0 -9999.000
    +120         20      6.37  -9999.00  -9999.00  -9999.00    -9999.0 -9999.000
    +121         21      4.04    320.41  -9999.00  -9999.00    -9999.0 -9999.000
    +122         22      5.51  -9999.00  -9999.00  -9999.00    -9999.0     0.825
    +123         23      4.80    293.72  -9999.00  -9999.00    -9999.0 -9999.000
    +125         25      5.13    304.41  -9999.00  -9999.00    -9999.0 -9999.000
                  0     0         0         0         0           0      0
  0         0           0         0         0         0           0      0
```

FIGURE D-8(a). Two hourly records from a QPMET file without editing of the data from the RAMSDAT file.

```
*TIMESET  9 191 1975
      +101           1    474.71   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +102           2  -9999.00   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +103           3  -9999.00   -9999.00   -9999.00   -9999.00        850.0     0.657
      +105           5      4.78   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +106           6      5.21   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +107           7      4.11   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +108           8      4.25   -9999.00   -9999.00   -9999.00        850.0     0.640
      +109           9      5.36   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +110          10      4.13   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +111          11  -9999.00   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +112          12      4.61   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +113          13      4.51   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +114          14      3.96   -9999.00   -9999.00   -9999.00        850.0     0.471
      +115          15      3.96   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +116          16      4.09   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +117          17      3.78   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +118          18      3.23   -9999.00   -9999.00   -9999.00        850.0     0.661
      +119          19      3.98   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +120          20      4.63   -9999.00       6.20     274.00        850.0 -9999.000
      +121          21      3.18   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +122          22      4.36   -9999.00   -9999.00   -9999.00        850.0    10.841
      +123          23      4.95   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +124          24  -9999.00   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +125          25      4.81   -9999.00   -9999.00   -9999.00        850.0 -9999.000
                     0         0          0          0          0            0         0
   701.000    4012.000  -9999.00     256.00   -9999.00   -9999.00      -9999.0 -9999.000
   654.900    4215.250  -9999.00   -9999.00   -9999.00   -9999.00       1050.0 -9999.000
         0           0         0          0          0          0            0         0
*TIMESET 10 191 1975
      +101           1    467.12     287.70   -9999.00   -9999.00        850.0 -9999.000
      +102           2  -9999.00     320.77   -9999.00   -9999.00        850.0 -9999.000
      +103           3      6.41     309.22   -9999.00   -9999.00        850.0     0.790
      +104           4      4.19     303.94       7.05     251.00        850.0     0.605
      +105           5      5.63     293.14   -9999.00   -9999.00        850.0 -9999.000
      +106           6      5.65     303.79   -9999.00   -9999.00        850.0 -9999.000
      +107           7      4.97     297.17   -9999.00   -9999.00        850.0 -9999.000
      +108           8      5.25     298.36   -9999.00   -9999.00        850.0     0.880
      +109           9      5.12   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +110          10      4.51     289.02   -9999.00   -9999.00        850.0 -9999.000
      +111          11  -9999.00   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +112          12      4.86   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +113          13      5.82     279.59   -9999.00   -9999.00        850.0 -9999.000
      +114          14      4.31     302.25   -9999.00   -9999.00        850.0     0.901
      +115          15      4.68     290.54   -9999.00   -9999.00        850.0 -9999.000
      +116          16      4.18     307.65   -9999.00   -9999.00        850.0 -9999.000
      +117          17      4.00     319.63   -9999.00   -9999.00        850.0 -9999.000
      +118          18      3.28     292.76   -9999.00   -9999.00        850.0     0.578
      +119          19      4.06     286.57   -9999.00   -9999.00        850.0 -9999.000
      +120          20      6.37   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +121          21      4.04     320.41   -9999.00   -9999.00        850.0 -9999.000
      +122          22      5.51   -9999.00   -9999.00   -9999.00        850.0    10.825
      +123          23      4.80     293.72   -9999.00   -9999.00        850.0 -9999.000
      +124          24  -9999.00   -9999.00   -9999.00   -9999.00        850.0 -9999.000
      +125          25      5.13     304.41   -9999.00   -9999.00        850.0 -9999.000
                     0         0          0          0          0            0         0
   654.900    4215.250  -9999.00   -9999.00       6.50     301.00       1050.0 -9999.000
   701.000    4012.000      7.10     256.00   -9999.00   -9999.00      -9999.0 -9999.000
         0           0         0          0          0          0            0         0
```

FIGURE D-8(b). Two hourly records from a QPMET file altered by the input file shown in Fig. D-6.

TABLE D-4. Format for QICON file.

Card Format	Information
(5X,E10.0)	Specifies Gaussian distance constant for interpolation.
(45X,F10.0)	Specifies reference height. These first two cards occur only once at the beginning of the file.
(38X,3(1X,I2))	Day, hour, and minute. This card begins each hourly data set.
(1X,A10,1X,4A10)	A pollutant record is begun by a -*POLLUTANT- card with the pollutant specified by name on the rest of the card.
(1X,A10)	The next card must contain the string -SURFACE-.
(1X,A10)	-STATION- indicates the beginning of station data.
(1X,A4,3X,I3,E15.0)	Station symbol, station number, and pollutant concentration. A zero or negative station number ends the station data set.
(1X,A10)	-UTM- indicates the beginning of UTM data.
(1X,2F10.0,E15.0)	UTM east coordinate, UTM north coordinate, and pollutant concentration. A zero or negative east coordinate ends the UTM data set.
(1X,A10)	-*ENDSET*- marks the end of an hourly data set.

```
USE     0.1000 AS THE GAUSSIAN DISTANCE CONSTANT FOR INTERPOLATION
REFERENCE HEIGHT OF OBSERVATIONS IN CM             100.
THE FOLLOWING DATA SET IS VALID UNTIL181? 0?00 (DAY?HOUR?MINUTE)
*POLLUTANT  OZONE
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
+101      1      2.50E-003
+102      2      2.50E-003
+103      3      2.50E-003
+104      4      2.50E-003
+105      5      2.50E-003
+106      6      2.50E-003
+107      7      2.50E-003
+108      8      2.50E-003
+109      9      2.50E-003
+110     10      2.50E-003
+111     11      2.50E-003
+112     12      7.72E-003
+113     13      1.89E-002
+114     14      2.50E-003
+115     15      2.50E-003
+116     16      2.50E-003
+117     17      2.50E-003
+118     18      9.04E-003
+119     19      2.55E-003
+120     20      4.32E-003
+121     21      2.43E-002
+122     22      1.91E-002
+124     24      1.29E-002
         0
UTM OBSERVATIONS
        0.
*POLLUTANT  CARBON MONOXIDE
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
+101      1      8.23E-001
+102      2      6.90E-001
+103      3      1.44E+000
+104      4      1.12E+000
+106      6      9.37E-001
+107      7      1.00E+000
+108      8      2.75E+000
+109      9      9.28E-001
+110     10      4.31E-001
+111     11      1.31E+000
+113     13      5.12E-001
+114     14      1.92E+000
+115     15      8.93E-001
+116     16      7.50E-001
+117     17      8.14E-001
+118     18      8.51E-002
+119     19      4.71E-001
+120     20      5.21E-001
+121     21      1.39E-001
+122     22      1.27E-001
+124     24      1.30E-001
+125     25      9.97E-002
         0
UTM OBSERVATIONS
        0.
*POLLUTANT  ALKENES
```

FIGURE D-9. Example of QICON header cards and one hourly record.

```
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
+101       1        1.73E-002
+104       4        2.80E-002
+106       6        1.11E-002
+107       7        9.57E-003
+108       8        2.73E-002
+109       9        7.46E-003
+110      10        2.49E-003
+111      11        7.22E-003
+113      13        1.31E-003
+114      14        1.46E-002
+115      15        5.96E-003
+116      16        5.72E-003
+117      17        1.16E-002
+119      19        1.11E-002
+120      20        3.40E-003
+121      21        2.22E-004
+122      22        2.00E-004
+124      24        2.00E-004
+125      25        2.00E-004
           0
 UTM OBSERVATIONS
          0.
 *POLLUTANT  ALKANES
 SURFACE   OBSERVATION DATA FOLLOWS
 STATION OBSERVATIONS
 +101       1        1.50E-001
 +104       4        2.43E-001
 +106       6        9.63E-002
 +107       7        8.32E-002
 +108       8        2.38E-001
 +109       9        6.49E-002
 +110      10        2.17E-002
 +111      11        6.28E-002
 +113      13        1.14E-002
 +114      14        1.27E-001
 +115      15        5.19E-002
 +116      16        4.98E-002
 +117      17        1.01E-001
 +119      19        9.66E-002
 +120      20        2.95E-002
 +121      21        1.93E-003
 +122      22        1.74E-003
 +124      24        1.74E-003
 +125      25        1.74E-003
            0
 UTM OBSERVATIONS
          0.
 *POLLUTANT  ALDEHYDES
 SURFACE   OBSERVATION DATA FOLLOWS
 STATION OBSERVATIONS
 +101       1        5.18E-003
 +104       4        8.39E-003
 +106       6        3.32E-003
 +107       7        2.87E-003
 +108       8        8.19E-003
 +109       9        2.24E-003
 +110      10        7.48E-004
 +111      11        2.17E-003
 +113      13        3.94E-004
 +114      14        4.39E-003
```

FIGURE D-9. Continued.

```
+115     15         1.79E-003
+116     16         1.72E-003
+117     17         3.47E-003
+119     19         3.33E-003
+120     20         1.02E-003
+121     21         6.66E-005
+122     22         6.00E-005
+124     24         6.00E-005
+125     25         6.00E-005
          0
UTM OBSERVATIONS
         0.
*POLLUTANT  NITRIC OXIDE
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
+101      1         1.04E-002
+102      2         1.01E-002
+103      3         6.71E-002
+104      4         3.51E-002
+105      5         2.50E-003
+106      6         6.91E-003
+107      7         1.10E-002
+108      8         8.96E-002
+109      9         4.52E-002
+110     10         1.76E-002
+111     11         3.71E-002
+112     12         8.52E-003
+113     13         2.50E-003
+114     14         4.61E-002
+115     15         7.94E-002
+116     16         1.45E-002
+117     17         1.00E-002
+118     18         2.50E-003
+119     19         1.47E-002
+120     20         2.50E-003
+121     21         2.50E-003
+122     22         2.50E-003
+124     24         2.63E-003
+125     25         2.50E-003
          0
UTM OBSERVATIONS
         0.
*POLLUTANT  NITROGEN DIOXIDE
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
+101      1         5.35E-002
+102      2         3.83E-002
+103      3         5.62E-002
+104      4         4.10E-002
+106      6         4.69E-002
+107      7         4.35E-002
+109      9         2.79E-002
+110     10         4.47E-002
+111     11         4.47E-002
+113     13         2.59E-002
+114     14         5.28E-002
+115     15         3.80E-002
+116     16         4.04E-002
+117     17         3.34E-002
+118     18         2.19E-002
+119     19         3.60E-002
+120     20         3.27E-002
```

FIGURE D-9. Continued.

```
+121     21       1.15E-002
+122     22       8.19E-003
+124     24       1.74E-002
+125     25       2.60E-003
          0
UTM OBSERVATIONS
         0.
*POLLUTANT  SULFUR DIOXIDE
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
+108      8       2.50E-003
          0
UTM OBSERVATIONS
         0.
*POLLUTANT  SULFATE
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
          0
UTM OBSERVATIONS
         0.
*POLLUTANT  NITROUS ACID
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
          0
UTM OBSERVATIONS
         0.
*POLLUTANT  NITRIC ACID
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
          0
UTM OBSERVATIONS
         0.
*POLLUTANT  HYDROGEN PEROXIDE
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
          0
UTM OBSERVATIONS
         0.
*POLLUTANT  ALKYL NITRITES
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
          0
UTM OBSERVATIONS
         0.
*ENDSET*
THE FOLLOWING DATA SET IS VALID UNTIL181? 1?00 (DAY?HOUR?MINUTE)
*POLLUTANT  OZONE
SURFACE   OBSERVATION DATA FOLLOWS
STATION OBSERVATIONS
+101      1       9.60E-003
+102      2       2.50E-003
+103      3       2.50E-003
+104      4       2.50E-003
+105      5       2.50E-003
+106      6       5.35E-003
+107      7       5.49E-003
+108      8       2.50E-003
+109      9       2.69E-003
+110     10       4.61E-003
+111     11       3.11E-003
+112     12       2.18E-002
+113     13       2.28E-002
```

FIGURE D-9. Continued.

APPENDIX E

M-PROCESSOR

DESCRIPTION

MASCON treats all meteorological data read from QMET as instantaneous measurements at the time of the QMET data set. MPROC assumes that the hourly timesets in QPMET represent either instantaneous measurements every hour on the half-hour or average values for the hour starting at the time-set time. Thus, a half-hour disparity exists between the data times as specified in QPMET and the instantaneous data times used in QMET. In addition, MPROC produces QMET data sets using a time interval between sets that is an integer number of hours. Therefore, in generating QMET files from the QPMET timesets, MPROC must average the QPMET data in a manner that best utilizes the QPMET data to obtain values representative of the QMET data-set times. To accomplish this, MPROC uses the linear weightings

$$
\begin{aligned}
w_i(t) &= \Delta t - |t - t_i - 0.5| \quad , \quad |t - t_i| < t \\
&= 0 \quad , \quad |t - t_i| \geq t \quad ,
\end{aligned}
$$

where:

t is a QMET data-set time,

Δt is the QMET data-set time interval in hours,

t_i is a QPMET time-set time,

and

$w_i(t)$ is the unnormalized weighting applied to the QPMET time set for t_i in generating the QMET data set for time t.

This weighting ensures that all values are interpolated to the QMET data-set times, and that, regardless of the QMET time interval, equal use is made of each QPMET time set when its contribution to all QMET data sets is summed. If values are missing, the average is computed from all values present. The averaging process for a given data item V at a location point P is given by

$$\dot{V}(t,P) = \sum_i w_i(t)\ V(t_i,P) \Big/ \sum_i w_i(t).$$

where the summation is made over all QPMET times t_i that have a nonzero weighting $w_i(t)$ and for which an observation $V(t_i,P)$ is available. If no values for a given data field are present with nonzero weighting for a given time and location, that field is omitted for that time and location. Each data field is sorted by location (either station number or UTM coordinates) before it is sent to QMET.

QMET

This file contains meteorological data formatted for input to the MASCON model. It is composed of meteorological-data time sets, each of which is divided into eight data-field subsets. Each time set begins with a header card containing the seven-character literal *METSET, as well as the hour, the Julian day of the year, and the year in which the data in the set are of maximum validity. The QMET file is terminated by an end-of-data card consisting of a header card with hour, Julian-day, and year fields set to minus one.

The eight data-field subsets of each main time set are: inversion-base heights specified at stations by station number, inversion-base heights specified at arbitrary locations by UTM easting-northing coordinate pairs, surface winds by station numbers, mean-layer winds and layer depths by station numbers, surface wind by UTM coordinates, mean-layer winds by UTM coordinates, atmospheric-column optical transmissivities by station numbers, and optical transmissivities by UTM coordinates. A header card containing an appropriate comment begins each data-field subset. An input record with a station number of zero terminates input to subsets. An input record with coordinates of zero terminates input to subsets in which locations are specified by UTM coordinates. A detailed description of the QMET file format appears in Table 7 of the MASCON User's Guide (Stullich, et al., 1978).

As control information to MPROC, the user supplies the start time, stop time, and time interval for the QMET data set. Start and stop times are specified by hour, Julian day, and year; the QMET time interval is specified as an integer number of hours. The default location for this information is in the file INPUT, following the logical record for system control cards. This location may be changed by specifying another file name on the system control card that executes MPROC. The format for the MPROC control information is shown in Table E-1.

TABLE E-1. Format for MPROC control information.

Card Format	Information
(6X,A2,1X,A3,1X,A4)	Start time (time of first QMET data set); hour of the day, Julian day of the year, and year.
(6X,A2,1X,A3,1X,A4)	Stop time (time of last QMET data set); hour of the day, Julian day of the year, and year.
(9X,I2)	Data-set output time interval in integer hours.

APPENDIX F

MASCON

The MASCON processor takes meteorological data, calculates flux fields from measured winds and inversion heights and interpolates these over the grid. It then adjusts these interpolated flux fields to attain mass consistency. These adjusted flux fields are then output in the form of QTRANx files for use by the LIRAQ models. The MASCON model is fully described in Stullich et al. (1979), and will not be discussed in detail here. We will give only a brief discussion of MASCON input and output files. Table F-1 lists MASCON input files. QMET is discussed in Appendix D and QGEO is discussed in Chapter 7.

QMRUN

QMRUN is the only user generated input file used by MASCON. The formats are described in Table F-2 and a sample is given in Fig. F-1.

The QMRUN file is a basic-run-specification file that spatially and temporally defines the problem being run and sets flags for several output options. Specifically, QMRUN identifies a problem being run in terms of the following:

1. A textual identification of the problem being run.
2. Initial and final time and date of the run.
3. The transfer coefficient or basic calculation interval.
4. Flux statistics flag.
5. Tabular-output selection flag.
6. Graphic-output selection flag.
7. The number of mesh intersections in the X and Y directions, the physical zone size, and the UTM coordinates of the lower-left corner of the modeling area.

A run may begin on any whole hour and extend for any integer number of hours, on any day of the year. Naturally, the amount of data provided in the QMET file should be consistent with the start and end times given in the QMRUN file.*

---

*MASCON will run before and after data periods by assuming persistence of meteorological conditions.

TABLE F-1. Summary of input files to MASCON.

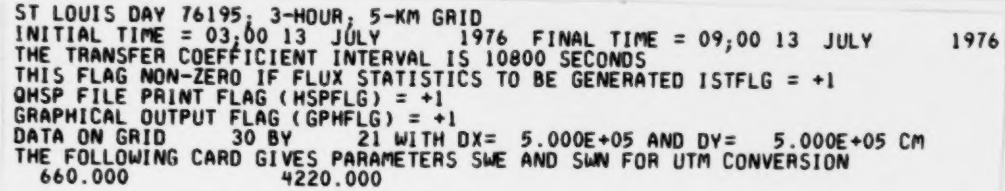
File name	Purpose	Contents
QMRUN	Basic problem specification	Problem identification, time limits, time interval, grid size and location.
QGEO	Topographic and geographic data	Topographic data, data points specifying geographic outlines, and station locations.
QMET	Meteorological data	Inversion-base height, wind data, and optical transmissivity.

TABLE F-2. Card-by-card format of the QMRUN file.

Card	Information
(4A10)	Problem identification. Limited to 40 characters.
(16X,2A10,A4,15X,2A10,A4)	Initial and final times/dates for the problem. Data must be left-justified within their fields, without abbreviation.
(38X,I5)	Transfer coefficient interval (seconds).
(65X,I1)	Flux statistics flag.
(33X,I2)	Tabular output flag.
(34X,I2)	Graphic output flag.
(15X,I5,5X,I5,10X,E10.3,10X,E10.3)	Number of grid squares in the X direction, Y direction, and grid sizes (cm).
. . .	. . .
(F10.0,10X,F10.0)	UTM coordinates (easting and northing) of southwest corner of the modeling area.

Although there is no theoretical limit to the length of the model simulation period, a practical limit of 48 h is reasonable. Since typical LIRAQ-2 runs require 45-60 min of computer time — central processing unit (CPU) plus input/output — per simulation day. MASCON runs are usually only made for periods up to 24 h.

Meteorological data may be entered with any integer number of hours as a data interval, but the basic calculation interval used is typically 1, 2, or 3 h, as specified



```
ST LOUIS DAY 76195, 3-HOUR, 5-KM GRID
INITIAL TIME = 03;00 13  JULY       1976  FINAL TIME = 09;00 13  JULY      1976
THE TRANSFER COEFFICIENT INTERVAL IS 10800 SECONDS
THIS FLAG NON-ZERO IF FLUX STATISTICS TO BE GENERATED ISTFLG = +1
QHSP FILE PRINT FLAG (HSPFLG) = +1
GRAPHICAL OUTPUT FLAG (GPHFLG) = +1
DATA ON GRID     30 BY     21 WITH DX=  5.000E+05 AND DY=   5.000E+05 CM
THE FOLLOWING CARD GIVES PARAMETERS SWE AND SWN FOR UTM CONVERSION
  660.000             4220.000
```

FIGURE F-1. Sample of a QMRUN file.

in the QMRUN file. This time must be less than or equal to the shortest interval between data entries. Transfer coefficients are generated at the middle of each calculation period and are assumed constant over the interval.

A flux-statistics flag can be set on or off (1 or 0, respectively) to control the generation of flux data at station locations (rather than at grid locations). If the flag is on, flux data are generated wherever possible to reflect pseudo-observed fluxes (wherever and whenever observed station winds are entered at both the beginning and end of a calculation period). This is done by using an interpolated inversion-base height from the grid back to the station. Fluxes are produced in terms of U and V components, as well as absolute magnitude. In addition, interpolated-unadjusted and mass-consistent adjusted fluxes are generated, so that comparisons can readily be made among all three flux types. In this way, numerical data are available at station locations to help the user determine the change in fluxes during the interpolation and the mass-consistent adjustment processes.

The tabular-output flag control the amount of tabular data accumulated in the QHSP and QDIAG files. The user can choose over a range, from minimal output to full detailed output, with some increase in cost, depending on choice. Options are:

-1 = minimal output

0 = standard output

+1 = detailed output .

The types of output are described under "Output files."

Similarly, the user has the choice of no graphic output, a standard graphic output package, or a detailed graphic display of several meteorological and mathematical fields that are useful for detailed diagnostic interpretation. This is controlled as follows by the graphic-output-flag option:

-1 = no graphics

0 = standard graphics

+1 = detailed graphics .

Since graphic output requires additional processing, the choice of detailed graphics can considerably increase the cost of a run.

The number of mesh intersections is limited by the memory available to MASCON. On the CDC 7600 at LBL, array sizes have been set rather high to accommodate previous users of the model. The domain treated must be rectangular and no larger than 66 x 66 mesh intersections (i.e., 65 x 65 zones). The offset point is arbitrary, as long as the bounds of the available topography specified in the QGEO file are not exceeded. The grid size may be any integer number of km; it must be the same in the X and Y directions without rotation of the mesh from geographic directions.*

The user must be careful in selecting start times, stop times, and data intervals for use with MASCON and the meteorological data preprocessor MPROC, so that inconsistent choices of these parameters do not produce unsatisfactory results or aborted runs.

In constructing a QMET file with MPROC, the user must specify the start and stop times of the data sets, as well as the time interval between sets. In constructing a QMRUN file, the user also specifies a start time, stop time, and output data interval for running MASCON. It is important to recognize that these times need not be the same as those stipulated with MPROC.

The MPROC code allows for more generality than the MASCON code, i.e., the user may select any time range of data and data interval in building the QMET file. Once he has made that choice, MASCON only allows the user to run with a start time that coincides with one of the data-set times included in the QMET file and with an output data interval of 1, 2, or 3 h. If the start time does not coincide with a data-set time in the QMET file, the code will abort before running very long.

The choice of a stop time is less restrictive; the output data interval will end on the last output data-set time immediately following the stop time. If the output data interval specified in the QMRUN file is not an even multiple of the input data interval used in the QMET file, the actual data output interval used by the code will not be constant, but will oscillate to ensure that an output data set does not span beyond an input data time.

The recommended approach is to construct the QMET and QMRUN files so that a model start time matches one of the data-set times, and the input and output data intervals are equal.

MASCON output files are listed in Table F-3. Samples of MASCON output are given in the microfiche addendum. Only the QTRANx files are used by the LIRAQ codes. These files must be stored on some archival medium if they are to be used by the LIRAQ codes. The QTRANx file formats are given in Table F-4 and portions of a sample are given in Fig. F-2.

QTRAN

The QTRAN file consists of a family of files: QTRAN0, QTRAN1, QTRAN2, . . . QTRAN9, QTRANA, QTRANB,* with (after two lines of identification in

---

*Simulations for the BAAQMD have been performed using grid sizes of 1, 2, and 5 km.

TABLE F-3. Summary of output files from a MASCON run.

File name	Purpose	Contents
DAYFILE	Record of computer run	Record of system control and staging information, including timing, charges, and fatal-error messages.
QDIAG	Diagnostic information	Code-detected error conditions and warnings.
QFLXCK	Statistical flux data	Flux data interpolated to station locations, including observed fluxes, interpolated inadjusted fluxes, and interpolated mass-consistent fluxes.
QHSP	Miscellaneous tabulated data	Topographic data, observed and interpolated meteorological data, boundary-condition type array, diffusivity coefficients, and mass-consistency checks.
QTRANx	Transfer coefficients for LIRAQ	Diffusivities, mass transfer coefficients, inversion-base heights, transmissivities, and source multiplier flags.
QGRAPH	Graphic analyses	Graphic plots of topography and input meteorological data, contour analyese of inversion-base heights and miscellaneous auxiliary quantities, and streamline plots of wind and flux fields.
OUTPUT	Record of run errors	Details of FORTRAN library error messages and graphics error messages

the first file) data for two complete time cycles per file. The data within a time cycle consists of three sections:

1. Surface vertical-eddy diffusivities,
2. Vertical and horizontal transfer coefficients for west, south, and top side of grid box,
3. Inversion-base heights, atmospheric transmissivities, and source-multiplier flags.

All of these variables, except the source-multiplier flags, are described fully in Chapter 8 of MacCracken and Sauter (1975). The source-multiplier flags indicate

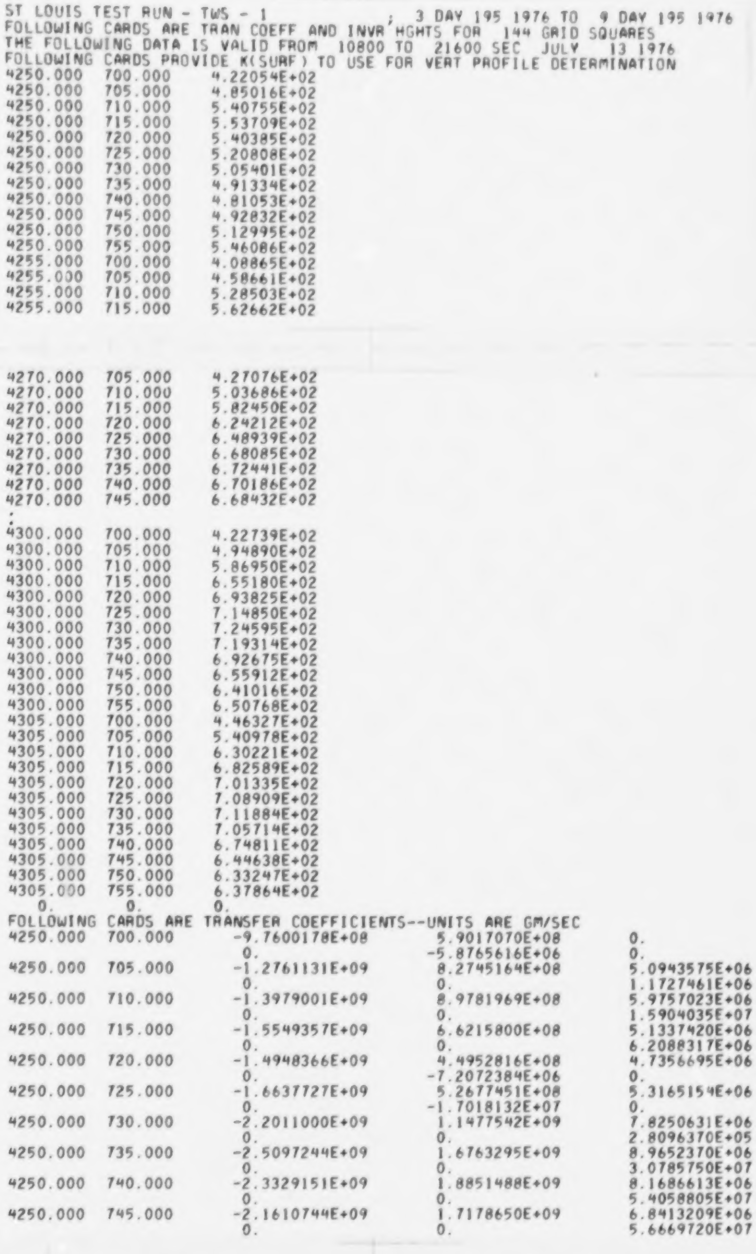
TABLE F-4. Format of the QTRAN file.

Card format	Variables	Description
(4A10,5X,A10,3X,2A10)	NAME,ID	Textual information identifying run, name, date, time, etc.
(51X,I5,13X)	NGDBX0	Indicates number of grid squares or zones over which problem was run. First two cards appear once; remainder of file format is repeated for each calculational cycle (here 3h).
(34X,I7,3X,I7,6X,A6,I3,A5)	TDT1,TDT2,IMN,IDAY1,IYR	Starting and ending hours and month/day/year between which following set of data is valid.
None	None	Text description. Begins data section giving vertical diffusion coefficient at surface.
(1X,2F9.3,E15.5)	UTMN,UTME,SFKZG	UTM-north, UTM-east lower left coordinates of zone where given-surface vertical-diffusion coefficient applies. Zero fields for UTM coordinates signal end of section. SFKZG is given in cm^2/s.
None	None	Text description.

TABLE F-4. Continued.

Card format	Variables	Description
(1X,2F9.3,3E20.7/19X,3E20.7)	UTMN,UTME,TRAN	Begins transfer coefficient data section. UTM-north, UTM-east, lower left coordinates of zone of following transfer coefficients. Note there are six TRAN values (two lines) per zone. Zero fields for UTM coordinates indicate end of section. Units of TRAN are g/s. The six TRAN values are X- and Y-direction advection fluxes, X- and Y-horizontal-eddy diffusion fluxes, flux from top of zone, and flux to top of zone. Horizontal fluxes are given for western and southern sides of the boxes and are positive toward east and north. Vertical fluxes are positive into box.
(65X,F15.2)	HINMIN	Minimum inversion-base height of zone. Applies if a zone has been omitted from list. Units are cm.
(1X,2F9.3,2F15.2,5X,F5.2,2X,F5.1)	UTMN,UTME,HINVR1G, HINVR2G,WOIK2,SRMTC	Begins section containing inversion-base heights and other data. UTM-north, UTM-east coordinates of zone of applicability; average inversion-base height (cm) at center of zone at beginning and end of period, atmospheric transmissivity value, and source-multiplier flag. Zero UTM-north value signals end of section.
Same as third card of table	Same as third card of table	Negative hour values signal end of QTRAN data.

that an individual grid cell is isolated from transport mechanisms acting in the subinversion well-mixed layer. This isolation occurs when the inversion base descends below topography and, thus, puts the region in the above-inversion layer. Under these conditions, the LIRAQ model does account for the pollutant source emissions into the isolated air volumn (for convenience, maintained at a 50-m thickness) associated with that grid square.



```
ST LOUIS TEST RUN - TWS - 1               ;  3 DAY 195 1976 TO  9 DAY 195 1976
FOLLOWING CARDS ARE TRAN COEFF AND INVR HGHTS FOR  144 GRID SQUARES
THE FOLLOWING DATA IS VALID FROM  10800 TO  21600 SEC  JULY   13 1976
FOLLOWING CARDS PROVIDE K(SURF) TO USE FOR VERT PROFILE DETERMINATION
4250.000  700.000     4.22054E+02
4250.000  705.000     4.85016E+02
4250.000  710.000     5.40755E+02
4250.000  715.000     5.53709E+02
4250.000  720.000     5.40385E+02
4250.000  725.000     5.20808E+02
4250.000  730.000     5.05401E+02
4250.000  735.000     4.91334E+02
4250.000  740.000     4.81053E+02
4250.000  745.000     4.92832E+02
4250.000  750.000     5.12995E+02
4250.000  755.000     5.46086E+02
4255.000  700.000     4.08865E+02
4255.000  705.000     4.58661E+02
4255.000  710.000     5.28503E+02
4255.000  715.000     5.62662E+02

4270.000  705.000     4.27076E+02
4270.000  710.000     5.03686E+02
4270.000  715.000     5.82450E+02
4270.000  720.000     6.24212E+02
4270.000  725.000     6.48939E+02
4270.000  730.000     6.68085E+02
4270.000  735.000     6.72441E+02
4270.000  740.000     6.70186E+02
4270.000  745.000     6.68432E+02
:
4300.000  700.000     4.22739E+02
4300.000  705.000     4.94890E+02
4300.000  710.000     5.86950E+02
4300.000  715.000     6.55180E+02
4300.000  720.000     6.93825E+02
4300.000  725.000     7.14850E+02
4300.000  730.000     7.24595E+02
4300.000  735.000     7.19314E+02
4300.000  740.000     6.92675E+02
4300.000  745.000     6.55912E+02
4300.000  750.000     6.41016E+02
4300.000  755.000     6.50768E+02
4305.000  700.000     4.46327E+02
4305.000  705.000     5.40978E+02
4305.000  710.000     6.30221E+02
4305.000  715.000     6.82589E+02
4305.000  720.000     7.01335E+02
4305.000  725.000     7.08909E+02
4305.000  730.000     7.11884E+02
4305.000  735.000     7.05714E+02
4305.000  740.000     6.74811E+02
4305.000  745.000     6.44638E+02
4305.000  750.000     6.33247E+02
4305.000  755.000     6.37864E+02
   0.        0.       0.
FOLLOWING CARDS ARE TRANSFER COEFFICIENTS--UNITS ARE GM/SEC
4250.000  700.000        -9.7600178E+08        5.9017070E+08        0.
                          0.                  -5.8765616E+06        0.
4250.000  705.000        -1.2761131E+09        8.2745164E+08        5.0943575E+06
                          0.                   0.                   1.1727461E+06
4250.000  710.000        -1.3979001E+09        8.9781969E+08        5.9757023E+06
                          0.                   0.                   1.5904035E+07
4250.000  715.000        -1.5549357E+09        6.6215800E+08        5.1337420E+06
                          0.                   0.                   6.2088317E+06
4250.000  720.000        -1.4948366E+09        4.4952816E+08        4.7356695E+06
                          0.                  -7.2072384E+06        0.
4250.000  725.000        -1.6637727E+09        5.2677451E+08        5.3165154E+06
                          0.                  -1.7018132E+07        0.
4250.000  730.000        -2.2011000E+09        1.1477542E+09        7.8250631E+06
                          0.                   0.                   2.8096370E+05
4250.000  735.000        -2.5097244E+09        1.6763295E+09        8.9652370E+06
                          0.                   0.                   3.0785750E+07
4250.000  740.000        -2.3329151E+09        1.8851488E+09        8.1686613E+06
                          0.                   0.                   5.4058805E+07
4250.000  745.000        -2.1610744E+09        1.7178650E+09        6.8413209E+06
                          0.                   0.                   5.6669720E+07
```

FIGURE F-2. Example of part of a QTRAN file.

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4250.000  750.000      -2.0583957E+09     1.2983188E+09     5.5272196E+06
                        0.                0.                3.3624693E+07
4250.000  755.000      -2.3054021E+09     1.0996788E+09     6.4446752E+06
                        0.                0.                1.5580760E+07
4250.000  760.000      -2.5607913E+09     0.                0.
                        0.                0.                0.
4255.000  700.000      -1.0568163E+09     6.0440196E+08     0.
                        4.0747886E+06    -3.2492201E+06     0.
4255.000  705.000      -1.3567868E+09     6.7039014E+08     4.8328656E+06
                        5.4227301E+06    -4.8666126E+06     0.
4255.000  710.000      -1.7171926E+09     7.9749172E+08     6.8749871E+06
                        6.2613143E+06     0.                1.2666312E+07
4255.000  715.000      -1.6240617E+09     3.4380933E+08     4.7740114E+06
                        5.1753930E+06    -7.5940378E+06     0.
4255.000  720.000      -1.6843215E+09     3.4532658E+08     5.4109085E+06
   :                    5.0249009E+06    -1.8899875E+07     0.
   :
4300.000  760.000      -2.9891012E+09     0.                0.
                        0.                0.                0.
4305.000  700.000      -2.3914382E+09     1.4203361E+09     0.
                        6.8260724E+06    -3.1353854E+07     0.
4305.000  705.000      -3.0299263E+09     2.0372742E+09     7.9337094E+06
                        8.9762541E+06    -5.6203910E+07     0.
4305.000  710.000      -3.7239730E+09     2.6141821E+09     1.0269866E+07
                        1.1573133E+07    -6.8826918E+07     0.
4305.000  715.000      -4.2822844E+09     3.0012705E+09     1.2726647E+07
                        1.3215213E+07    -5.5654932E+07     0.
4305.000  720.000      -4.2317813E+09     2.7944549E+09     1.2794740E+07
                        1.3532744E+07    -3.9709115E+07     0.
4305.000  725.000      -3.9170326E+09     2.2635792E+09     1.2305417E+07
                        1.3106815E+07    -2.0284943E+07     0.
4305.000  730.000      -3.5825444E+09     1.8395771E+09     1.1463130E+07
                        1.1882532E+07    -3.2033895E+06     0.
4305.000  735.000      -3.1902153E+09     1.4299853E+09     1.0242122E+07
                        1.0784309E+07     0.                5.6736374E+06
4305.000  740.000      -2.9669070E+09     1.1098576E+09     9.8998990E+06
                        9.9784631E+06     0.                1.9665311E+07
4305.000  745.000      -2.5729783E+09     5.7928206E+08     8.1572629E+06
                        9.0254428E+06     0.                1.9719668E+07
4305.000  750.000      -2.4650624E+09     3.3415691E+08     8.0450874E+06
                        8.2006085E+06     0.                2.5617913E+07
4305.000  755.000      -2.3620498E+09     1.8213288E+08     7.0942177E+06
                        7.6173875E+06     0.                1.6872913E+07
4305.000  760.000      -2.5186299E+09     0.                0.
                        0.                0.                0.
4310.000  700.000       0.                1.7674500E+09     0.
                        0.                0.                0.
4310.000  705.000       0.                2.4350160E+09     0.
                        0.                0.                0.
4310.000  710.000       0.                2.8786427E+09     0.
                        0.                0.                0.
4310.000  715.000       0.                2.6684654E+09     0.
                        0.                0.                0.
4310.000  720.000       0.                2.1975241E+09     0.
                        0.                0.                0.
4310.000  725.000       0.                1.6459927E+09     0.
                        0.                0.                0.
4310.000  730.000       0.                1.1624529E+09     0.
                        0.                0.                0.
4310.000  735.000       0.                9.1559403E+08     0.
                        0.                0.                0.
4310.000  740.000       0.                4.2744142E+08     0.
                        0.                0.                0.
4310.000  745.000       0.                1.7472873E+08     0.
                        0.                0.                0.
4310.000  750.000       0.               -6.5360136E+07     0.
                        0.                0.                0.
4310.000  755.000       0.                2.8386419E+07     0.
                        0.                0.                0.
4310.000  760.000       0.                0.                0.
                        0.                0.                0.
   0.        0.         0.                0.                0.
                        0.                0.                0.
FOLLOWING ARE INVERSION HEIGHTS(CM), IF NOT GIVEN ASSUMED TO BE        5000.00
4250.000  700.000      7337.38       17587.93       .72     1.0
4250.000  705.000      8652.31       18903.36       .72     1.0
4250.000  710.000      7221.62       17225.33       .72     1.0
4250.000  715.000      5412.35       15093.53       .72     1.0
4250.000  720.000      5952.86       15687.94       .71     1.0
   :
   :
4300.000  745.000     13882.77       24510.21       .79     1.0
4300.000  750.000     12030.00       23122.90       .81     1.0
4300.000  755.000      9479.25       21015.89       .82     1.0
4305.000  700.000     15462.02       24981.37       .72     1.0
4305.000  705.000     17568.31       26358.45       .72     1.0
4305.000  710.000     20178.62       28416.80       .71     1.0
4305.000  715.000     20976.24       29273.8        .70     1.0
```

FIGURE F-2. Continued.

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4305.000  720.000        19387.21        28264.22        .69    1.0
4305.000  725.000        17197.17        26818.86        .68    1.0
4305.000  730.000        14474.74        24783.90        .69    1.0
4305.000  735.000        12680.54        23544.89        .70    1.0
4305.000  740.000        11071.06        22352.62        .72    1.0
4305.000  745.000         9729.58        21311.49        .74    1.0
4305.000  750.000         8714.75        20507.72        .76    1.0
4305.000  755.000         7435.85        19414.70        .76    1.0
   0.        0.              0.              0.          0.     0.
THE FOLLOWING DATA IS VALID FROM  21600 TO  32400 SEC  JULY   13 1976
FOLLOWING CARDS PROVIDE K(SURF) TO USE FOR VERT PROFILE DETERMINATION
4250.000  700.000    6.34043E+02
4250.000  705.000    6.74920E+02
4250.000  710.000    6.94530E+02
4250.000  715.000    6.92485E+02
4250.000  720.000    6.79984E+02
4250.000  725.000    6.65266E+02
4250.000  730.000    6.52808E+02
4250.000  735.000    6.40796E+02
4250.000  740.000    6.30358E+02
4250.000  745.000    6.40642E+02
4250.000  750.000    6.67218E+02
4250.000  755.000    7.01887E+02
4255.000  700.000    6.24610E+02
4255.000  705.000    6.67286E+02
4255.000  710.000    6.95184E+02
4255.000  715.000    7.00706E+02
4255.000  720.000    6.89171E+02
4255.000  725.000    6.72960E+02
4255.000  730.000    6.59787E+02
4255.000  735.000    6.46967E+02
4255.000  740.000    6.38756E+02
4255.000  745.000    6.53217E+02
4255.000  750.000    6.83647E+02
4255.000  755.000    7.21613E+02
4260.000  700.000    6.17421E+02
4260.000  705.000    6.61519E+02
4260.000  710.000    6.98276E+02
4260.000  715.000    7.12325E+02
4260.000  720.000    7.04872E+02
4260.000  725.000    6.88188E+02
4260.000  730.000    6.73840E+02
4260.000  735.000    6.64541E+02
4260.000  740.000    6.54305E+02
4260.000  745.000    6.65465E+02
4260.000  750.000    7.03564E+02
4260.000  755.000    7.52435E+02
4265.000  700.000    6.13467E+02
4265.000  705.000    6.58050E+02
4265.000  710.000    7.02293E+02
4265.000  715.000    7.27189E+02
4265.000  720.000    7.25560E+02
4265.000  725.000    7.11130E+02
4265.000  730.000    6.98288E+02
4265.000  735.000    6.89812E+02
.
.
.
4295.000  735.000        29491.56        41157.85        .74    1.0
4295.000  740.000        28894.53        42049.02        .74    1.0
4295.000  745.000        28087.71        42703.05        .75    1.0
4295.000  750.000        26390.62        42258.77        .76    1.0
4295.000  755.000        23517.87        40576.46        .76    1.0
4300.000  700.000        24422.55        41259.02        .74    1.0
4300.000  705.000        26981.32        42422.15        .73    1.0
4300.000  710.000        29619.89        43218.03        .72    1.0
4300.000  715.000        31587.17        43724.61        .72    1.0
4300.000  720.000        32145.87        43925.06        .72    1.0
4300.000  725.000        30307.09        42757.55        .72    1.0
4300.000  730.000        27619.88        41265.64        .73    1.0
4300.000  735.000        26196.07        41147.87        .73    1.0
4300.000  740.000        25296.29        41438.06        .74    1.0
4300.000  745.000        24510.21        41631.45        .74    1.0
4300.000  750.000        23122.90        40989.74        .75    1.0
4300.000  755.000        21015.89        39592.77        .75    1.0
4305.000  700.000        24981.37        41437.05        .74    1.0
4305.000  705.000        26358.45        41383.26        .74    1.0
4305.000  710.000        28416.80        42218.83        .74    1.0
4305.000  715.000        29273.86        42899.34        .73    1.0
4305.000  720.000        28264.22        42673.69        .73    1.0
4305.000  725.000        26818.86        42361.54        .72    1.0
4305.000  730.000        24783.90        41405.30        .72    1.0
4305.000  735.000        23544.89        41047.45        .73    1.0
4305.000  740.000        22352.62        40520.76        .73    1.0
4305.000  745.000        21311.49        39959.98        .73    1.0
4305.000  750.000        20507.72        39494.15        .74    1.0
4305.000  755.000        19414.70        38698.64        .74    1.0
   0.        0.              0.              0.          0.     0.
THE FOLLOWING DATA IS VALID FROM  -1000 TO  -1000 SEC  JULY   13 1976
```

FIGURE F-2. Continued.

BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
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APPENDIX G

LIRAQ-1S

LIRAQ-1 is described in detail in the 1975 LIRAQ reports (MacCracken and Sauter, 1975) and the 1975 LIRAQ Users Guide (MacCracken, 1975). No changes were made in the internal logic of LIRAQ-1, but several changes have been made in input and output files. Most of these changes are comparatively minor and are associated with the use of Julian dates, although one diagnostic file, QTYM, has been added to the output.

LIRAQ-1S simulates the evolution of regional air quality as a result of the effects of transport and simple source/sink events. It can treat simple linear loss processes, but cannot incorporate nonlinear chemical interactions. LIRAQ-1S uses input information on topography, meteorology, initial pollutant fields, source rates, and various run specifications (e.g., period to be simulated, details of simulation grid). As output it generates regional patterns of air quality including spatial and temporal variations (in both graphical and tabular form) and it generates a record of the computational time steps.

Table G-1 gives the input files associated with LIRAQ-1S. The remainder of this appendix discusses those files.

TABLE G-1. Input files associated with LIRAQ-1S.

Filename	Content	Where Generated	Where described in detail
QGEO	Topographic data	Archived on data cell	Chapter 7
QICON	Initial pollutant concentrations	QPROC	Appendix D
QSRUN	Run parameters	User	Below
QSORxx	Source emission data	SORPROC	Appendix A
QTRANx	Meteorological data	MASCON	MASCON Users Guide below

LIRAQ-1S INPUT FILES

LIRAQ-1S input files are functionally the same as the files described in MacCracken (1975). There are several comparatively minor differences in file format, however. Extensive changes in QGEO, the topographic data file are described in Chapter 7. One simple, but pervasive, change affecting QTRANx, QSORxx, QICON and QSRUN is that all of these files now contain a Julian or calendar date that is used by the code. In the earlier version of LIRAQ-1, calendar date appeared in the QTRANx files but was only used for titling. Days appearing in QICON and QSRUN referred to day from start of data set, and QSOR was dated only by season and year. Now, however, all of these files contain dates, and all are used. Care must be taken to ensure that all dated files refer to the same date. QICON, QTRANx, and QSRUN will always contain a date and must agree. QSORxx can contain either a true Julian date or can be assigned a Julian date of 000. If the date in QSORxx is nonzero it must agree with QSRUN, etc. If the date in QSORxx is zero, the QSORxx file will not be treated as a date specific file and it need not agree with QSRUN, QICON, and QTRANx.

TREC1 is the interval between keeping data at stations in the QSREC file. It should be set to 00:30 if VERF is to be used.

TMBAL is the time inverval between mass balance computations. 03:00 to 01:00 are reasonable values.

QSRUN

QSRUN is the only user-generated LIRAQ-1 input file. Figure G-1 gives an example and Table G-2 provides a description of the input formats. The only changes to the content or format of QSRUN information for LIRAQ-1 made since 1975 are in the cards that input TIN, TFIN, TDLITE, TPINT, TREC1, and TMBAL. All of these cards have been converted from 3(1X,I2) format to 2(1X,I2), 5X, I3, 1X,I4 to convert

```
LIRAQ1S; DAY 76195; INT5; 5 KM; R1003
LIRAQ 5 KM GRID    660.  810. 4220. 4320.
09?00 DAY 195 1976  INITIAL TIME
15?00 DAY 195 1976  FINAL TIME
00?00               DAYLIGHT SAVING TIME SHIFT
01?00               PRINT INTERVAL
00?30               TIME HISTORY RECORD INTERVAL
03?00               MASS BALANCE INTERVAL
THE FOLLOWING STATIONS WILL HAVE TIME HISTORIES KEPT
  1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
 21  22  23  24  25 000
THE FOLLOWING UTM LOCATIONS WILL HAVE TIME HISTORIES KEPT
0.        0.0
  1 CARBON MONOXIDE
SOURCE COLUMN AND MULTIPLIERS                              7  1.0000E+00  1.0000E+00
MOLECULAR WEIGHT     28.00
BACKGROUND VALUES  W .1100E+00 E .1100E+00 S .1100E+00 N .1100E+00 A .1100E+00
  2 SULFUR DIOXIDE
SOURCE COLUMN AND MULTIPLIERS                              6  1.0000E+00  1.0000E+00
MOLECULAR WEIGHT     64.00
BACKGROUND VALUES  W 1.000E-02 E 1.000E-02 S 1.000E-02 N 1.000E-02 A 1.000E-02
  0
```

FIGURE G-1. Example of a LIRAQ-1S QSRUN file.

TABLE G-2. Format of QSRUN data cards.

Card No.	Columns	Format	Symbol	Units	Value limits	Typical value	Description
1	1–40	4A10	NAME	—	—	LIRAQ-1S, Day 195, INT 5, 5 km, run 100	Problem name
2	7–8	I2	DX	km	1,2,3,4,5,...	1,2, or 5	Grid size
2	19–24	F6.0	UTME1	km	In area covered by QGEO	660	UTM easting coordinate of west edge of domain
2	25–30	F6.0	UTME2	km	In area included in QGEO	810	UTM easting coordinate of east edge of domain
2	31–36	F6.0	UTMN1	km	In area included in QGEO	4220	UTM northing coordinate of south edge of domain
2	37–42	F6.0	UTMN2	km	In area included in QGEO	4320	UTM northing coordinate of north edge of domain
3*	2–3,5–6 12–14, 16–19	2(1X,I2),5X I3,1X,I4	TIM	hr:min	Day, year must agree with QTRANx, QICON file and emissions file (if day not 000 in emissions file).	01:00 195 1976 simulation	Start time of model simulation

*This format has changed since the 1975 version of LIRAQ-1.

TABLE G-2. Continued.

Card No.	Columns	Format	Symbol	Units	Value limits	Typical value	Description
4*	2-3,5-6, 12-14, 16-19	2(1X,I2),5X I3,1X,I4	TFIN	hr:min	Must agree with QTRANx, QICON and emissions file (if day not 000 in emissions file)	21:00 195 1976 simulation	Final time of model simulation
5*	2-3,5-6	2(1X,I2),5X, I3,1X,I4	TDLITE	hr:min	00:00 or 01:00	01:00	Shift from daylight time to standard time
6*	2-3,5-6	2(1X,I2),5X, I3,1X,I4	TPINT	hr:min	00:30 to 03:00	01:00	Time interval between printed output of data
7*	2-3,5-6	2(1X,I2),5X, I3,1X,I4	TRECI	hr:min	00:15 to 03:00	00:30	Time interval between keeping of data for station histories
8*	2-3,5-6,	2(1X,I2),5X, I3,1X,I4	TMBAL	hr:min	01:00 to 24:00	03:00	Time interval between mass balance calculations
9	—	—	—	—	—	—	Descriptive card
10,11	1-80	20I4	NSTHL	—	Station Nos. 1 to NMAX; 0 indicates no further data	43	Station numbers indicating stations at which to keep time histories
12	—	—	—	—	—	—	Descriptive card

TABLE G-2. Continued.

Card No.	Columns	Format	Symbol	Units	Value limits	Typical value	Description
13	1-80	10F8.0	LOCHST	Set of pairs of UTM coordinates	Within QGEO	690 4240	UTM location at which station history is to be kept
14	1-4	I4	NPL	—	1 to 4	1	Pollutant number
14	5-44	4A10	NTIT	Hollerith	—	Carbon Monoxide	Pollutant name
15	51-54	I4	KLMSOR	—	1,2,3,4,5,6 or 7	7	Column in QSOR file in which pollutant emissions to be found
15	55-66, 67-78	2E12.4	SORMUL	—	none	1.0	Source multipliers to convert units or modify source
16	20-27	F8.0	AMOL	grams per mole	Depends on pollutant	28 pollutant	Molecular weight of
17	20-79	5(2X,E10.3)	PBKGL	ppm	None, but should not create excessively sharp gradients	0.11,0.11,0.11, 0.11,0.11 east, south, north and	Boundary concentrations for pollutant on west, above domain
18-21	Repeat of cards 14 to 17 for second pollutant (optional)						
22-25	Repeat of cards 14 to 17 for third pollutant (optional)						
26-29	Repeat of cards 14 to 17 for fourth pollutant (optional)						
30	—	—	—	—	0	0	Indicator at end of QSRUN file

from day (of simulation:hour of day:minute to hour of day:minute Julian day year information. Only TIN and TFIN actually use the day and year information, but care should be taken to ensure that columns 12-19 are blank on cards 5-8.

The name is a title of convenience. The name in the example provided in Fig. G-1 gives the ARCHIVE address we used for a particular debugging run.

DX must be the same as that given in the QTRANx and QSORxx files. If it is not the same as in QTRANx the code will attempt to run but will abort. If DX is different from the grid interval for emissions the code will abort (emissions grid finer than LIRAQ grid) or run expensively and uselessly (emissions grid coarser than LIRAQ grid.

The values of UTME1, UTME2, UTMN1, and UTMN2 should all lie within the grid covered by QGEO (and QTRANx) and should cover an area slightly larger than the area of primary interest. In the interests of economy DX should be large and the grid should be kept to the minimum that covers all source and receptor regions of interest. However, fidelity to observation should improve if DX is smaller and the grid more extensive.

TIN and TFIN establish the time interval to be simulated. Care should be taken that the years and the Julian dates are the same.

TDLITE is 00:00 if standard time is used in the emissions inventories, 01:00 if Daylight Savings time is used in the emissions inventories.

TPINT is the interval between printed output data. If one is simulating over a period of several hours to a day, 01:00 is a convenient interval.

NSTHL can contain any station numbers identified in QGEO up to a limit of 40 stations. VERF will only be given correct sites if no more than 25 stations are used. LOCHST can contain up to 10 UTM coordinate pairs. If VERF is to be used, UTM coordinate pairs count in the limit of 25 stations.

NPL is a number to be associated with a particular pollutant. In LIRAQ-1S if one pollutant is to be simulated NPL should be 1, if two pollutants are to be simulated NPL should be 1 for the first, 2 for the second and so forth up to a limit of four pollutants. NTIT is a pollutant name and must have the spelling associated with that pollutant in Q1ICON.

KLMSOR is the column in the emissions files (QSORxx) associated with a given pollutant. KLMSOR can vary from 1 to 7. Column 1 is normally particulates, 2 is alkanes, 3 is alkenes, 4 is aldehydes, 5 is nitric oxide, 6 is sulphur dioxide, and 7 is carbon monoxide.

SORMUL is a multiplier that can be used to correct units (so that the nominal ppmV units are numerically equal to $\mu g/m^3$ for example). AMOL is a molecular weight, and PBGKL are boundary conditions (in ppmV).

QGEO

QGEO gives map data and topographic data. It is fully described in Chapter 7 of this report. QGEO for St. Louis is stored in data cell directory MASCON and can be obtained by executing the command:

```
FETCHPS, MASCON, QGEO, QGEOSTL.
```

A QGEO for the San Francisco area is stored in the same directory with the name QGEOSFB. Anyone wishing to use the LIRAQ codes in a different region will need to generate a QGEO for that region.

The St. Louis QGEO covers the UTM coordinates from 654E to 813E, from 4213N to 4330N. This is a smaller area than is covered by the RAPS grid.

QICON

QICON is generated by the Q processor, QPROC. The format content and procedure for generation are described in Appendix D.

QTRANx

QTRANx files are generated by MASCON. Their generation is described in detail in the MASCON Users Guide (Stullich, et al., 1979).

QSORxx

QSOR is generated by the source processor. The formats, content procedures for generating QSORxx are described in Appendix A.

LIRAQ-1 OUTPUT FILES

LIRAQ-1 generates the five output files listed in Table G-3.

QHSP

The major LIRAQ-1S tabular output file is QHSP. A sample of QHSP content is given in Fig. G-2. QHSP echos most input. It also contains tables of computed mixing ratios over the entire grid. It identifies the sources and sinks of pollutant mass (e.g., emissions, initial conditions inflow and outflow, deposition to the ground) for each grid element and for the entire grid. And it displays the mass fluxes of various pollutants at each grid cell.

QGRAPH

QGRAPH presents a graphical display of pollutant concentrations both as computed 1 meter above the surface and averaged over the mean layer. These plots are contour diagrams superimposed on a map. It also contains a plot of pollutant concentration vs. time for the stations selected in QSRUN. Figures G-3 through G-5 are samples of QGRAPH output.

QSREC

QSREC contains the computed concentrations of pollutants at the stations specified in QSRUN. Figure G-6 is an example of QSREC output. The formats are given in Table G-4. QSREC is used by the verification routine VERF. If VERF is to

TABLE G-3. Output files associated with LIRAQ-1S.

Filename	Content	Use	Where described in detail
OUTPUT	Diagnostic error messages	Diagnostic	LBL Users Manual
QTYM	LIRAQ-1S time step length	Diagnostic	Below
QSREC	Computed concentrations at selected stations	Verification	Below
QHSP	Tabular output - run parameters (initial time), species characteristics (initial), initial conditions, surface average concentrations (periodic), vertical average concentrations (periodic), ratio of surface to vertical average concentrations (periodic), pollutant mass balances (periodic), meteorological data (periodic), pollutant fluxes (periodic)	interpolation of air quality	Below
QGRAPH	Inversion base height (periodic), surface concentration (periodic), vertical average concentrations (periodic), station and UTM history concentrations	Interpolation of air quality	Below
DAYFILE	Summary extention	Diagnosis and accounting	LBL Users Manual

be run, TREC1 should be set to 00:30 in QSRUN, and the total number of stations and UTM locations at which concentrations are to be recorded should not exceed 25.

QTYM

QTYM gives the LIRAQ-1 time steps. An example is given in Fig. G-7. In the normal course of events, QTYM will be of little interest to the user. However, if a LIRAQ-1 problem requires an abnormal amount of CPU time, examination of QTYM may reveal the source of any problems. The time steps in LIRAQ-1 are determined as the lesser of 300 seconds, or $(1/2)(\Delta x/u)$ or $(1/2)(\Delta y/v)$ where $\Delta x = \Delta y$, is the LIRAQ grid interval, u or v is the highest velocity component in the x or y direction in any grid cell. If the LIRAQ-1 time step is abnormally small this suggests a high flux velocity. Abnormally high velocities imply either that the LIRAQ and MASCON grids are incompatible, or that the QTRANx files contain an abnormally high flow velocity. Because the inversion heights vary over a meteorological time interval, but not the mass fluxes, the internally deduced velocities can exceed realistic velocities by as

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TYPING GUIDE SHEET

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TOP OF IMAGE AREA

CHAPTER HEAD, BEGIN SECTIONS HERE

```
LIRAQ1S; DAY 76195; INT3; 5 KM; R1002


LIRAQ 5 KM GRID    720.  810. 4220. 4320.


 INITIAL TIME ...............    6; 0 DAY 195 1976
 FINAL TIME .................    7; 0 DAY 195 1976
 DAYLIGHT SAVING OFFSET .....    0; 0 DAY
 PRINT INTERVAL .............    1; 0 DAY
 TIME HISTORY RECORD INTERVAL    0;30 DAY
 MASS BALANCE EDIT INTERVAL      3; 0 DAY


TIME HISTORIES WILL BE KEPT AT THE FOLLOWING  23 STATIONS


  1   740.000  4275.000 +101      1
  2   740.000  4285.000 +102      2
  3   745.000  4280.000 +103      3
  4   745.000  4275.000 +104      4
  5   740.000  4275.000 +105      5
  6   735.000  4275.000 +106      6
  7   740.000  4280.000 +107      7
  8   745.000  4290.000 +108      8
  9   755.000  4275.000 +109      9
 10   745.000  4270.000 +110     10
 11   735.000  4270.000 +111     11
 12   730.000  4280.000 +112     12
 13   735.000  4285.000 +113     13
 14   740.000  4295.000 +114     14
 15   755.000  4295.000 +115     15
 16   760.000  4290.000 +116     16
 17   760.000  4270.000 +117     17
 18   740.000  4260.000 +118     18
 19   725.000  4270.000 +119     19
 20   720.000  4285.000 +120     20
 21   730.000  4300.000 +121     21
 22   775.000  4285.000 +123     23
 23   745.000  4235.000 +124     24


TIME HISTORIES WILL BE KEPT AT THE FOLLOWING   0 EXPLICIT UTM LOCATIONS


POLLUTANTS TO BE RUN]


   1 CARBON MONOXIDE
   2 SULFUR DIOXIDE


MASS FLUXES (GM-AIR/SEC) FROM       0 TO    10800  ON JULY   13 1976
  EASTING NORTHING     XADV         YADV          XDIF          YDIF          TPOUT       TPIN

  720.000 4220.000  -.5334E+09  -.2785E+08  0.            0.            -.1045E+08  0.
  725.000 4220.000  -.6076E+09  -.1241E+08   .2811E+07    0.            -.1060E+08  0.
  730.000 4220.000  -.6736E+09   .4266E+08   .3091E+07    0.            -.9354E+07  0.
  735.000 4220.000  -.8764E+09   .2162E+09   .4087E+07    0.            -.1255E+07  0.
  740.000 4220.000  -.9914E+09   .2123E+09   .3798E+07    0.            -.3790E+07  0.
  745.000 4220.000  -.1231E+10   .3232E+09   .4628E+07    0.            -.3087E+07  0.
  750.000 4220.000  -.1222E+10   .2790E+09   .4458E+07    0.            -.4607E+07  0.
  755.000 4220.000  -.1012E+10   .6294E+08   .3521E+07    0.            -.1172E+08  0.
  760.000 4220.000  -.9107E+09  -.6835E+08   .3252E+07    0.            -.1749E+08  0.
  765.000 4220.000  -.1061E+10   .2876E+08   .4034E+07    0.            -.1494E+08  0.
  770.000 4220.000  -.1171E+10   .1036E+09   .4293E+07    0.            -.1058E+08  0.
  775.000 4220.000  -.1192E+10   .1586E+09   .4333E+07    0.            -.6623E+07  0.
  780.000 4220.000  -.1181E+10   .9436E+08   .4050E+07    0.            -.8989E+07  0.
  785.000 4220.000  -.1206E+10   .7031E+08   .4278E+07    0.            -.9150E+07  0.
  790.000 4220.000  -.1265E+10  -.1737E+08   .4170E+07    0.            -.1536E+08  0.
  795.000 4220.000  -.1439E+10   .1091E+09   .5282E+07    0.            -.9296E+07  0.
  800.000 4220.000  -.1401E+10  -.6772E+07   .4720E+07    0.            -.1368E+08  0.
  805.000 4220.000  -.1505E+10   .7396E+08   .5584E+07    0.            -.7824E+07  0.
  810.000 4220.000  -.1436E+10  0.           0.           0.            0.          0.
```

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BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS

FIGURE G-2. Sample of QHSP output from LIRAQ-1. Several hundred pages of similar output have been omitted.

PAGE NUMBER

EPA-287 (Cin.)
(4-76)

```
INVERSION HEIGHT ABOVE TOPO (M)
THE TIME IS NOW    6.00000 HOURS
   720.000 4315.000  .878E+02  .697E+02  .619E+02  .671E+02  .574E+02  .546E+02  .576E+02  .530E+02 .501E+02 .528E+02
   770.000 4315.000  .541E+02  .513E+02  .500E+02  .500E+02  .500E+02  .514E+02  .514E+02  .500E+02
   720.000 4310.000  .144E+03  .116E+03  .998E+02  .968E+02  .759E+02  .694E+02  .706E+02  .611E+02 .549E+02 .572E+02
   770.000 4310.000  .563E+02  .523E+02  .523E+02  .500E+02  .500E+02  .501E+02  .529E+02  .561E+02
   720.000 4305.000  .192E+03  .173E+03  .147E+03  .129E+03  .113E+03  .991E+02  .886E+02  .768E+02 .692E+02 .636E+02
   770.000 4305.000  .608E+02  .575E+02  .539E+02  .500E+02  .510E+02  .511E+02  .569E+02  .603E+02
   720.000 4300.000  .250E+03  .226E+03  .191E+03  .168E+03  .152E+03  .138E+03  .119E+03  .973E+02 .805E+02 .682E+02
   770.000 4300.000  .650E+02  .631E+02  .560E+02  .522E+02  .524E+02  .526E+02  .601E+02  .625E+02
   720.000 4295.000  .280E+03  .271E+03  .244E+03  .223E+03  .207E+03  .190E+03  .165E+03  .131E+03 .995E+02 .773E+02
   770.000 4295.000  .728E+02  .735E+02  .662E+02  .582E+02  .555E+02  .569E+02  .661E+02  .709E+02
   720.000 4290.000  .268E+03  .285E+03  .290E+03  .286E+03  .283E+03  .265E+03  .230E+03  .189E+03 .142E+03 .104E+03
   770.000 4290.000  .933E+02  .935E+02  .817E+02  .651E+02  .613E+02  .654E+02  .740E+02  .800E+02
   720.000 4285.000  .236E+03  .270E+03  .306E+03  .328E+03  .342E+03  .333E+03  .300E+03  .254E+03 .200E+03 .153E+03
   770.000 4285.000  .131E+03  .121E+03  .101E+03  .835E+02  .821E+02  .855E+02  .900E+02  .951E+02
   720.000 4280.000  .201E+03  .255E+03  .305E+03  .339E+03  .363E+03  .363E+03  .340E+03  .295E+03 .239E+03 .192E+03
   770.000 4280.000  .166E+03  .147E+03  .123E+03  .108E+03  .107E+03  .110E+03  .109E+03  .113E+03
```

```
MASS FLUXES (GM-AIR/SEC) FROM    21600 TO    32400  ON JULY   13 1976
  EASTING NORTHING      XADV          YADV          XDIF          YDIF          TPOUT         TPIN


   720.000 4220.000   -.3494E+10    .5058E+10  0.              0.            0.             .9602E+08
   725.000 4220.000   -.3529E+10    .5118E+10   .1247E+08  0.                0.             .9662E+08
   730.000 4220.000   -.3517E+10    .5178E+10   .1242E+08  0.                0.             .9698E+08
   735.000 4220.000   -.3806E+10    .5299E+10   .1337E+08  0.                0.             .1023E+09
   740.000 4220.000   -.4022E+10    .5185E+10   .1284E+08  0.                0.             .8588E+08
   745.000 4220.000   -.4393E+10    .5383E+10   .1391E+08  0.                0.             .7249E+08
   750.000 4220.000   -.4251E+10    .5133E+10   .1372E+08  0.                0.             .6224E+08
   755.000 4220.000   -.3779E+10    .4610E+10   .1258E+08  0.                0.             .5233E+08
   760.000 4220.000   -.3609E+10    .4464E+10   .1243E+08  0.                0.             .4755E+08
   765.000 4220.000   -.3985E+10    .4855E+10   .1385E+08  0.                0.             .5239E+08
   770.000 4220.000   -.4284E+10    .5071E+10   .1478E+08  0.                0.             .6005E+08
   775.000 4220.000   -.4529E+10    .5206E+10   .1536E+08  0.                0.             .6597E+08
   780.000 4220.000   -.4721E+10    .5172E+10   .1546E+08  0.                0.             .6240E+08
   785.000 4220.000   -.4945E+10    .5151E+10   .1620E+08  0.                0.             .6094E+08
   790.000 4220.000   -.5239E+10    .5153E+10   .1630E+08  0.                0.             .4573E+08
   795.000 4220.000   -.5610E+10    .5281E+10   .1788E+08  0.                0.             .4531E+08
   800.000 4220.000   -.5622E+10    .4863E+10   .1698E+08  0.                0.             .2618E+08
```

```
INVERSION HEIGHT ABOVE TOPO (M)
THE TIME IS NOW    6.00000 HOURS
   720.000 4315.000  .180E+03  .176E+03  .176E+03  .186E+03  .169E+03  .165E+03  .177E+03  .171E+03 .164E+03 .170E+03
   770.000 4315.000  .174E+03  .165E+03  .159E+03  .155E+03  .156E+03  .169E+03  .168E+03  .162E+03
   720.000 4310.000  .249E+03  .226E+03  .213E+03  .213E+03  .191E+03  .186E+03  .191E+03  .182E+03 .176E+03 .179E+03
   770.000 4310.000  .177E+03  .171E+03  .170E+03  .162E+03  .162E+03  .169E+03  .172E+03  .174E+03
   720.000 4305.000  .281E+03  .269E+03  .249E+03  .237E+03  .225E+03  .214E+03  .206E+03  .196E+03 .189E+03 .184E+03
   770.000 4305.000  .182E+03  .179E+03  .174E+03  .167E+03  .168E+03  .172E+03  .178E+03  .182E+03
   720.000 4300.000  .321E+03  .303E+03  .275E+03  .261E+03  .252E+03  .245E+03  .231E+03  .212E+03 .198E+03 .187E+03
   770.000 4300.000  .185E+03  .184E+03  .177E+03  .173E+03  .173E+03  .174E+03  .182E+03  .184E+03
   720.000 4295.000  .341E+03  .330E+03  .308E+03  .295E+03  .289E+03  .281E+03  .263E+03  .237E+03 .210E+03 .191E+03
   770.000 4295.000  .189E+03  .192E+03  .186E+03  .178E+03  .176E+03  .177E+03  .187E+03  .192E+03
   720.000 4290.000  .328E+03  .335E+03  .339E+03  .338E+03  .343E+03  .334E+03  .309E+03  .278E+03 .239E+03 .209E+03
   770.000 4290.000  .203E+03  .206E+03  .197E+03  .182E+03  .178E+03  .183E+03  .191E+03  .197E+03
   720.000 4285.000  .301E+03  .320E+03  .349E+03  .369E+03  .385E+03  .383E+03  .359E+03  .323E+03 .279E+03 .242E+03
   770.000 4285.000  .228E+03  .224E+03  .207E+03  .192E+03  .191E+03  .195E+03  .199E+03  .203E+03
```

```
THE GAUSSIAN INTERPOLATION CONSTANT IS     .1000E+00
AT LEAST  3 DATA POINTS WILL BE SOUGHT WITHIN A RADIUS OF  20 GRID ELEMENTS


REFERENCE HEIGHT OF OBSERVATIONS (CM)     .1000E+03
```

FIGURE G-2. Continued.

```
POLLUTANT  CARBON MONOXIDE
SOURCE COLUMN  7
MOLECULAR WEIGHT     28.00
BACKGROUND VALUES]  WEST      .1100E+00 EAST      .1100E+00
  SOUTH    .1100E+00 NORTH    .1100E+00 TOP       .1100E+00




 THE FOLLOWING  20 STATION OBSERVATIONS WERE WITHIN THE GRID


   1  +101     1      744.180 4279.860     .88900E+00
   2  +102     2      742.520 4286.050     .11800E+00
   3  +103     3      747.590 4282.470     .16000E+00
   4  +105     5      743.710 4276.450     .50000E-01
   5  +106     6      738.660 4277.570     .38300E+00
   6  +107     7      740.180 4282.610     .86500E+00
   7  +108     8      748.410 4291.100     .14800E+00
   8  +109     9      755.800 4279.890     .55300E-01
   9  +111    11      738.810 4272.480     .22600E+00
  10  +112    12      733.940 4280.910     .66100E+00
  11  +113    13      737.740 4289.820     .72800E+00
  12  +114    14      744.320 4297.460     .18700E+00
  13  +115    15      757.110 4297.800     .45100E+01
  14  +117    17      760.560 4272.820     .12800E+00
  15  +118    18      743.070 4263.260     .50000E-01
  16  +119    19      729.760 4270.550     .41700E+00
  17  +120    20      723.080 4285.910     .24300E+00
  18  +121    21      732.410 4302.380     .29400E+00
  19  +123    23      777.320 4286.380     .13300E+00
  20  +124    24      749.280 4236.540     .24200E+00



 THE FOLLOWING   0 UTM OBSERVATIONS WERE WITHIN THE GRID
```

```
SURFACE STATION OBSERVATIONS CONVERTED TO AVERAGE


   1  +101     1      744.180 4279.860     .35560E+00
   2  +102     2      742.520 4286.050     .47200E-01
   3  +103     3      747.590 4282.470     .64000E-01
   4  +105     5      743.710 4276.450     .20000E-01
   5  +106     6      738.660 4277.570     .15320E+00
   6  +107     7      740.180 4282.610     .34600E+00
   7  +108     8      748.410 4291.100     .59200E-01
   8  +109     9      755.800 4279.890     .22120E-01
   9  +111    11      738.810 4272.480     .90400E-01
  10  +112    12      733.940 4280.910     .26440E+00
  11  +113    13      737.740 4289.820     .29120E+00
  12  +114    14      744.320 4297.460     .74800E-01
  13  +115    15      757.110 4297.800     .47622E+01
  14  +117    17      760.560 4272.820     .51200E-01
  15  +118    18      743.070 4263.260     .20000E-01
  16  +119    19      729.760 4270.550     .16680E+00
  17  +120    20      723.080 4285.910     .97200E-01
  18  +121    21      732.410 4302.380     .23224E+00
  19  +123    23      777.320 4286.380     .99703E-01
  20  +124    24      749.280 4236.540     .22981E+00
```

```
RATIO OF SURF CON TO AVG CON - - TOTAL TO SURF PATH
720.000 4220.000        2.084     1.997     1.264     1.236      .981      .979     1.017     1.020     1.146     1.125
770.000 4220.000         .980      .985      .987     1.753     1.139     1.109      .948      .949
720.000 4225.000        2.500     1.665     1.153     1.149      .967      .967      .962      .963     1.188      .959
770.000 4225.000         .982     1.032     1.051     1.502     1.060     1.038      .949      .950
720.000 4230.000         .954     2.500      .959      .967      .964      .963      .963     1.026     1.576     1.058
770.000 4230.000        1.053     1.010     1.010     1.062     1.074     1.358      .950      .951
720.000 4235.000         .955     2.500      .967      .972      .965     1.061     1.060     1.066     1.033     1.031
770.000 4235.000        1.012     1.012     1.141     1.141      .992     1.014      .994      .994
720.000 4240.000         .956     2.232     1.053     1.025     1.019     1.079     1.073     1.004     1.040     1.039
770.000 4240.000        1.019     1.021     1.177     1.195     1.010     1.023      .994      .994
720.000 4245.000        1.007     2.500     1.550     1.061     1.052     1.989     1.070      .985     1.262     1.065
770.000 4245.000        1.571     1.028     1.281     1.326     1.091     1.086     1.045     1.044
```

FIGURE G-2. Continued.

```
    SURF CONCEN CONTOURS OF      CARBON MONOXIDE
THE TIME IS NOW    6.00000 HOURS
  720.000 4315.000  .133E+00  .155E+00  .156E+00  .338E+00  .660E+00  .837E+00  .114E+01  .128E+01 .135E+01 .113E+01
  770.000 4315.000  .813E+00  .552E+00  .274E+00  .168E+00  .127E+00  .115E+00  .112E+00  .114E+00
  720.000 4310.000  .201E+00  .313E+00  .228E+00  .483E+00  .106E+01  .168E+01  .193E+01  .251E+01 .282E+01 .294E+01
  770.000 4310.000  .268E+01  .205E+01  .133E+01  .677E+00  .326E+00  .177E+00  .121E+00  .156E+00
  720.000 4305.000  .208E+00  .205E+00  .196E+00  .183E+00  .111E+01  .205E+01  .254E+01  .271E+01 .302E+01 .287E+01
  770.000 4305.000  .258E+01  .191E+01  .123E+01  .691E+00  .390E+00  .233E+00  .130E+00  .156E+00
```

```
     AVG CONCEN CONTOURS OF      SULFUR DIOXIDE
THE TIME IS NOW    6.00000 HOURS
  720.000 4315.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01 .100E-01 .100E-01
  770.000 4315.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01
  720.000 4310.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01 .100E-01 .100E-01
  770.000 4310.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01
  720.000 4305.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01 .100E-01 .100E-01
  770.000 4305.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01
```

```
    SURF CONCEN CONTOURS OF      SULFUR DIOXIDE
THE TIME IS NOW    6.00000 HOURS
  720.000 4315.000  .641E-02  .640E-02  .637E-02  .635E-02  .649E-02  .643E-02  .629E-02  .630E-02 .637E-02 .640E-02
  770.000 4315.000  .646E-02  .674E-02  .669E-02  .675E-02  .677E-02  .676E-02  .679E-02  .683E-02
  720.000 4310.000  .638E-02  .651E-02  .642E-02  .648E-02  .651E-02  .641E-02  .627E-02  .625E-02 .636E-02 .652E-02
  770.000 4310.000  .661E-02  .665E-02  .672E-02  .676E-02  .675E-02  .675E-02  .676E-02  .690E-02
  720.000 4305.000  .634E-02  .634E-02  .636E-02  .634E-02  .668E-02  .692E-02  .658E-02  .634E-02 .642E-02 .655E-02
  770.000 4305.000  .664E-02  .667E-02  .674E-02  .677E-02  .678E-02  .675E-02  .675E-02  .688E-02
```

```
MASS DISTRIBUTION OF  CARBON MONOXIDE                          AT     6.0000 HOURS

TOTAL MASS IS      .89162E+09 GRAMS

 720.000 4220.000     .6192E+06   .7157E+06   .8809E+06   .1019E+07   .1136E+07   .1233E+07   .1122E+07 .9688E+06
 760.000 4220.000     .9394E+06   .9210E+06   .8353E+06   .7370E+06   .6828E+06   .6590E+06   .6821E+06 .6860E+06
 800.000 4220.000     .6688E+06   .6705E+06
 720.000 4225.000     .7424E+06   .1200E+07   .1519E+07   .1603E+07   .1517E+07   .1340E+07   .1220E+07 .1268E+07
 760.000 4225.000     .1406E+07   .1446E+07   .1381E+07   .1149E+07   .8910E+06   .7425E+06   .6865E+06 .6662E+06
 800.000 4225.000     .6397E+06   .6430E+06
```

```
MASS BALANCE IN GRAMS OF  CARBON MONOXIDE
FROM   6.0000 HOURS UNTIL   7.0000 HOURS

  E     N      CHANGE   =  XADV    +    YADV  +    XDIF   +    YDIF   +  TOPOUT +  TOPIN   +  BOTOUT +  SOURCE + CHEMLOSS

 720. 4220.   .287E+06   .110E+05  -.664E+04  -.20E-01   .59E+00  0.          .40E+05  -.31E+05   .27E+06  0.
 725. 4220.   .203E+06  -.964E+04  -.701E+05  -.36E-01   .10E+01  0.          .41E+05  -.32E+05   .27E+06  0.
 730. 4220.   .287E+05   .194E+06  -.280E+06   .17E+00   .12E+01  0.          .41E+05  -.19E+05   .93E+05  0.
 735. 4220.  -.710E+05   .131E+06  -.390E+06  -.94E-01   .14E+01  0.          .43E+05  -.19E+05   .16E+06  0.
 740. 4220.  -.197E+06   .239E+06  -.473E+06   .43E-01   .14E+01  0.          .36E+05  -.13E+05   .14E+05  0.
 745. 4220.  -.259E+06  -.414E+05  -.248E+06  -.31E-01   .13E+01  0.          .30E+05  -.14E+05   .14E+05  0.
 750. 4220.  -.205E+06  -.288E+06   .442E+05  -.12E+00   .98E+00  0.          .26E+05  -.15E+05   .28E+05  0.

 785. 4315.  -.224E+05  -.138E+07   .131E+07   .40E+01   .38E+01  0.          .47E+05  -.18E+05   .20E+05  0.
 790. 4315.   .178E+06  -.334E+06   .470E+06   .16E+01   .18E+01  0.          .39E+05  -.14E+05   .17E+05  0.
 795. 4315.   .240E+06   .432E+05   .159E+06   .49E+00   .43E+00  0.          .34E+05  -.13E+05   .18E+05  0.
 800. 4315.   .253E+06   .384E+05   .180E+06   .46E-01   .39E-01  0.          .30E+05  -.13E+05   .18E+05  0.
 805. 4315.   .248E+06   .744E+05   .145E+06   .17E-01   .14E+00  0.          .17E+05  -.13E+05   .25E+05  0.

REGIONAL SUMMARY - TOTAL MASS IS    .9738E+09 GRAMS


 .822E+08  -.184E+08  -.109E+09   .29E-12  -.33E-10  0.         .28E+08  -.18E+08   .20E+09  0.
```

FIGURE G-2. Continued.

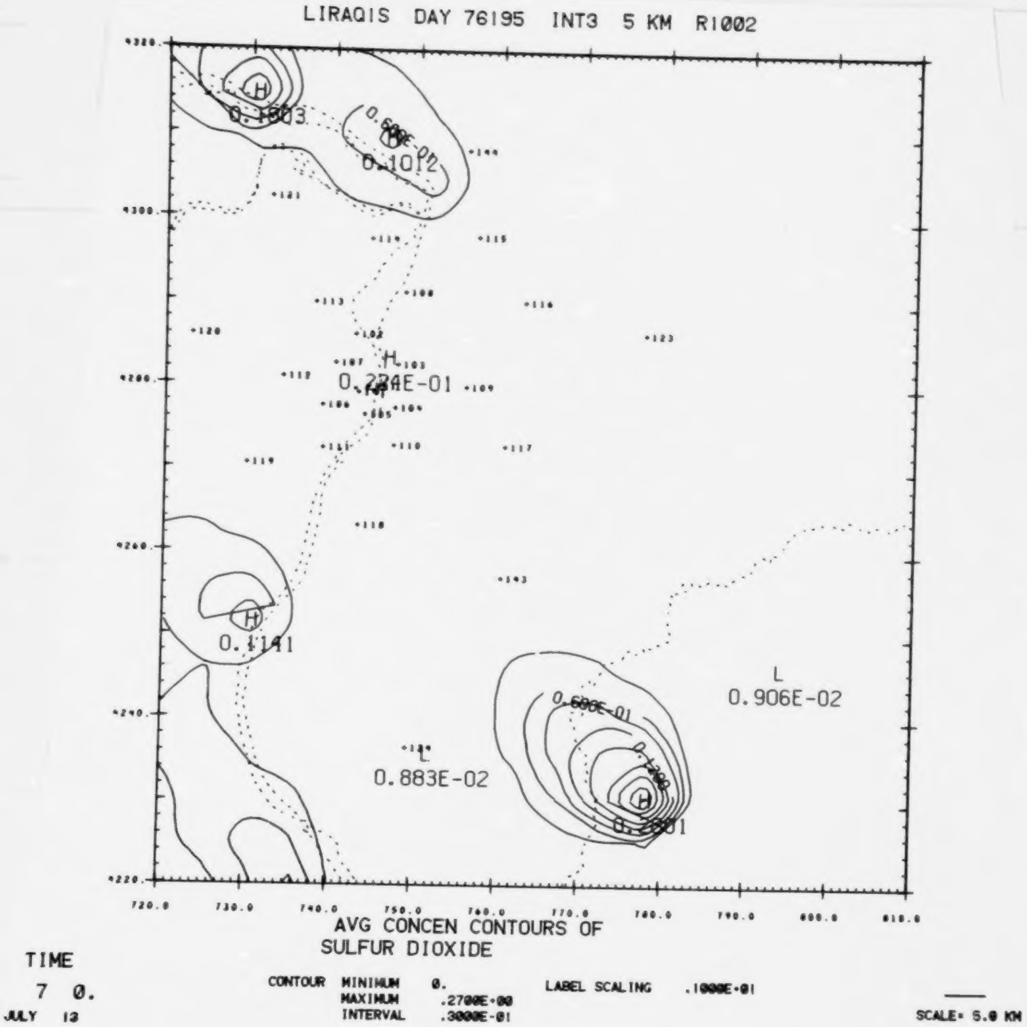

FIGURE G-3. Sample mean layer concentration plot from LIRAQ-1S.

much as an order of magnitude. However, time steps below 10 seconds suggest bad input unless the actual winds are quite strong during a period of rapidly changing mixing depth. It might occasionally be desirable to modify MASCON input to avoid this problem. The occasions for such editing might include bad input data to MASCON (e.g., a key punching error) or regions where the interpolation of mixing depth over topography produces an implausible flow pattern.

OUTPUT

The short file OUTPUT consists of messages sent by the FORTRAN libraries and compilers and default output from various LBL utility routines. It contains diagnostic error messages, information about changes in data cell files and the like. Minor

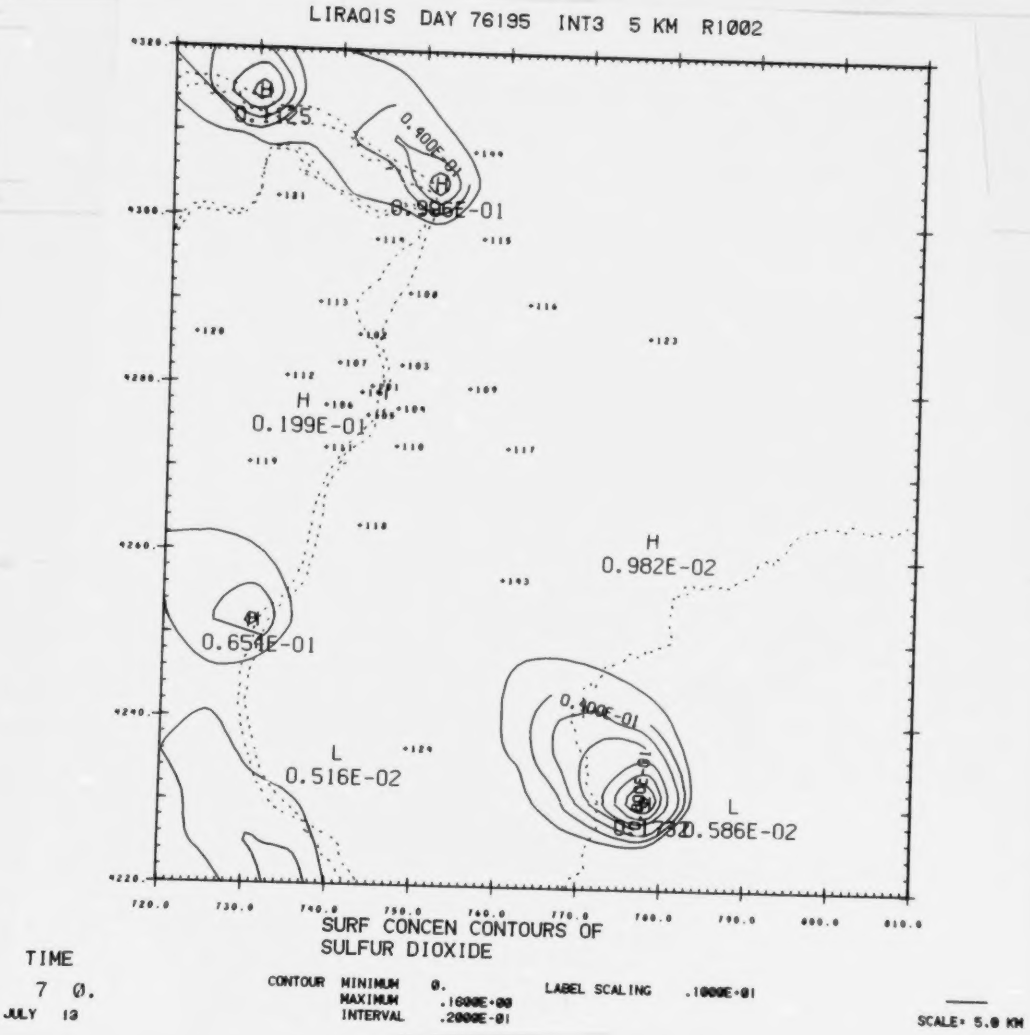

FIGURE G-4. Sample surface concentration plot from LIRAQ-1S.

changes in LBL graphics routines can generate substantial numbers of error messages that may not be reflected in the output.

Control Card Decks

The file DAYFILE is generated by the LBL system and describes the progress of the job through the system. This file can be very useful in determining the source of problems involved in running LIRAQ (e.g., a change in LBL systems routines such as TV80TLB or a bad address for an input file, or hardware problems such as inability to read a tape).

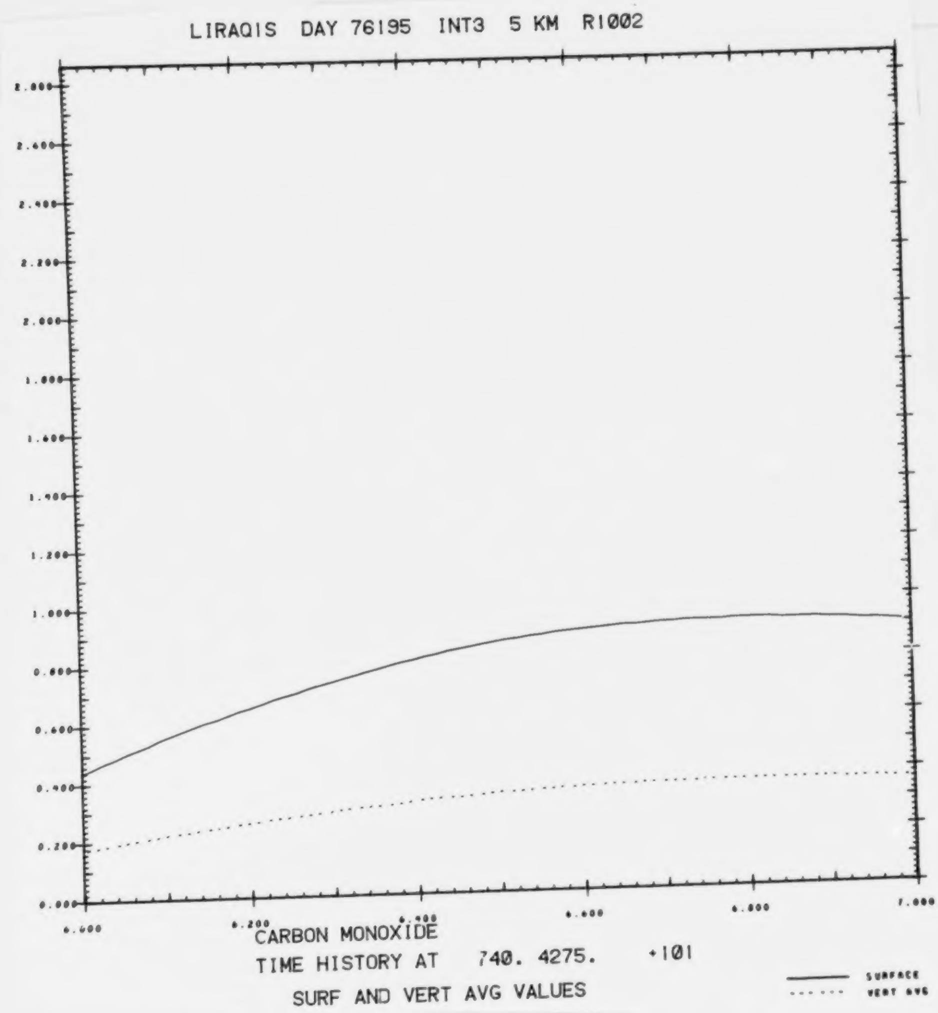

FIGURE G-5. Sample time history plot from LIRAQ-1S.

```
   LIRAQ1
LIRAQ1S; DAY 76195; INT3; 5 KM; R1002
  23     0    23    3         .60000E+01         .70000E+01         .50000E+00
   1        CARBON MONOXIDE
   0.                    .28631E+01
   1       +101     740. 4275.
        .1752E+00     .3461E+00     .3610E+00
        .4381E+00     .8652E+00     .9025E+00
   2       +102     740. 4285.
        .2216E+00     .2758E+00     .2924E+00
        .5539E+00     .6896E+00     .7310E+00
   3       +103     745. 4280.
        .1362E+00     .1230E+00     .1656E+00
        .3404E+00     .3074E+00     .4140E+00
   4       +104     745. 4275.
        .1472E+00     .1375E+00     .1795E+00
        .3681E+00     .3438E+00     .4488E+00
   5       +105     740. 4275.
        .1752E+00     .3461E+00     .3610E+00
        .4381E+00     .8652E+00     .9025E+00
   6       +106     735. 4275.
        .1691E+00     .3934E+00     .4892E+00
        .4227E+00     .9836E+00     .1223E+01
   7       +107     740. 4280.
        .2065E+00     .3131E+00     .3281E+00
        .5162E+00     .7826E+00     .8203E+00
   8       +108     745. 4290.
        .1000E+00     .6590E+00     .5398E+00
        .2501E+00     .1052E+01     .9169E+00
   9       +109     755. 4275.
        .8397E-01     .1100E+00     .1487E+00
        .2099E+00     .2749E+00     .3716E+00
  10       +110     745. 4270.
        .1176E+00     .9905E-01     .1340E+00
        .2940E+00     .2476E+00     .3350E+00

        .3985E+00     .6923E+00     .8056E+00
  20       +120     720. 4285.
        .1689E+00     .3431E+00     .5209E+00
        .4222E+00     .8577E+00     .1302E+01
  21       +121     730. 4300.
        .2053E+00     .2736E+00     .4988E+00
        .2686E+00     .3570E+00     .5649E+00
  23       +123     775. 4285.
        .5091E+00     .1747E+00     .1150E+00
        .5218E+00     .2140E+00     .1560E+00
  24       +124     745. 4235.
        .2150E+00     .2123E+00     .1928E+00
        .2282E+00     .2329E+00     .2131E+00
   2        SULFUR DIOXIDE
   0.                    .26855E-01
   1       +101     740. 4275.
        .1000E-01     .1479E-01     .1641E-01
        .1108E-01     .1468E-01     .1690E-01
   2       +102     740. 4285.
        .1000E-01     .1556E-01     .1865E-01
        .7867E-02     .1150E-01     .1355E-01
   3       +103     745. 4280.
        .1000E-01     .2007E-01     .2238E-01
        .9200E-02     .1582E-01     .1733E-01
   4       +104     745. 4275.
        .1000E-01     .1565E-01     .1654E-01
        .1123E-01     .1491E-01     .1567E-01
   5       +105     740. 4275.
        .1000E-01     .1479E-01     .1641E-01
        .1108E-01     .1468E-01     .1690E-01
   6       +106     735. 4275.
        .1000E-01     .1286E-01     .1521E-01
        .1552E-01     .1781E-01     .1991E-01
   7       +107     740. 4280.
        .1000E-01     .1683E-01     .1941E-01
        .8808E-02     .1353E-01     .1615E-01
```

FIGURE G-6. Sample of QSREC output from LIRAQ-1S. Several lines of similar output have been omitted.

```
CYCLE *        1      T =     21600.00      DLT =         .30000E+03
CYCLE *        2      T =     21900.00      DLT =         .30000E+03
CYCLE *        3      T =     22200.00      DLT =         .30000E+03
CYCLE *        4      T =     22500.00      DLT =         .30000E+03
CYCLE *        5      T =     22800.00      DLT =         .30000E+03
CYCLE *        6      T =     23100.00      DLT =         .30000E+03
CYCLE *        7      T =     23400.00      DLT =         .30000E+03
CYCLE *        8      T =     23700.00      DLT =         .30000E+03
CYCLE *        9      T =     24000.00      DLT =         .30000E+03
CYCLE *       10      T =     24300.00      DLT =         .30000E+03
CYCLE *       11      T =     24600.00      DLT =         .30000E+03
CYCLE *       12      T =     24900.00      DLT =         .30000E+03
```

FIGURE G-7. QTYM output from LIRAQ-1S.

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TABLE G-4. QSREC file format.

Card	Format	Description	Variables
1	IX,A10	Dropfile name	I60B(44B)
2	IX,4A10	Run title	NAME
3	4I5,3E15.5	NSTHST, number of labelled stations NUTHMH, number of stations given by UTMs NHIST, Total number of stations NCONL, number of entries stored XB1, start time in hours XB2, stop time in hours XDX, time interval in hours	NSTHST, NUTHMH, NHIST, NCONL, XB1 XB2, XDX
4	1X,I4,5X, 4A10	Pollutant number, pollutant name, lower & upper limits of pollutant concentration for plots.	NPL, NTIT, YCON1 YCON2
5	1X,I4,5X, A4,1X,1F6.0	Station number, station symbol, station UTMs	NSX, NSYM, UTME(IX), UTMN(JX)
6	4X,6E12.4	Average concentration	CON1(I), I=1,NCONL
7	4X,6E12.4	Surface concentration	CON1(I), I=1,NCONL
5-7	Repeat for each station.		
4-7	Repeat for each pollutant.		

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PAGE NUMBER

APPENDIX H

LIRAQ-2S

LIRAQ-2S closely resembles the code described in MacCracken and Sauter (1975) and MacCracken (1975). The changes in the internal workings of the code are described in Sections 2, 3, 6, and 7 of this report. Many of the changes were caused by the incorporation of SO_2 and $SO_4^=$ species and the associated changes in model chemistry. Other changes reflect a more versatile graphics routine, and the use of Julian dates. The chemical mechanism reflects the mid-1976 state-of-the-art. As such it is somewhat dated in 1979. However, since it was partially tuned against smog chamber results, the photochemical model retains whatever validity it originally had as a chamber simulation model. Viewed as such, the model should be an adequate interpolation device and a somewhat risky extrapolation tool.

The input files associated with LIRAQ-2S are listed in Table H-1. The files QGEO, QTRANx, QSORxx, and QICON are identical for LIRAQ-1S and LIRAQ-2S. The files QREST and QRAD are not used by LIRAQ-1S, while the file QSRUN serves the same purpose in LIRAQ-1S and LIRAQ-2S, but differs in its content.

INPUT FILES

QSRUN

Figure H-1 gives an example of QSRUN for LIRAQ-2S, Table H-2 gives the formats. As in the case of LIRAQ-1S (Appendix G), card 1 provides a title, card 2 sets the grid interval and domain, cards 3-8 set the start time, stop time, shift the emissions by one hour if the emissions are done in Daylight Savings Time, set the time between printed data output, between output to QSREC, and between mass balance calculations. LIRAQ-2S input differs from LIRAQ-1S input in that UTME2-UTME1 and UTMN2-UTMN1 must be equal to 20*DX, and in that TIMBAL is not used (although a card of the correct format must be present) since LIRAQ-2S does not compute mass balances. Card 9 is descriptive, cards 10 and 11 input station numbers at which time histories are to be kept, card 12 is descriptive, and card 13 identifies UTM locations at which records of pollutant concentrations are to be kept.

If the routine VERF is to be used to compare RAPS data with LIRAQ computations the sum of the number of stations and the UTM locations at which records are kept should not exceed 25.

Cards 14-17 give a pollutant number, NPL, and name, NTIT, the column in QSORxx from which emissions of the pollutant in question are to be taken, KLMSOR, (0 if there are no emissions for a particular species), SORMUL a multiplier that can

TABLE H-1. Input files associated with LIRAQ-2S.

Filename	Content	Tape reference #	Where generated	Where discussed
QGEO	Topographic and map data	9	Archived on data cell	Chapter 7
QICON	Initial pollutant concentrations	8	Q-Processor	Appendix D
QSORxx	Source emissions data	5	Source processor	Appendix A
QSRUN	Run parameters	10	User	Below
QTRANx	Meteorological data	22	MASCON	MASCON Users Guide and Appendix F
QRAD	Photodissociation rate coefficients as a function of cosine of the solar zenith angle	13	Archived on data cell	Below
QREST	(Optional) concentrations of all species at each grid element	6	LIRAQ-2S	Below

be used to split emissions between various species (e.g., 10% of NO emissions might be assigned to NO_2), AMOL, the molecular weight, and PBKGL, minimum pollutant concentrations to be used at boundaries.

Cards 18-61 repeat these cards for 11 other pollutants. In LIRAQ-2S, unlike LIRAQ-1S there is a definite list of 12 pollutants that must be treated by cards 14-61.

Cards 14-17 deal with species 1, alkenes, KLMSOR = 3, AMOL = 44, PBGKL typically in the range of 5×10^{-3} to 6×10^{-2} ppmV.

Cards 18-21 deal with species 2, alkanes, KLMSOR=2, AMOL=58, PBGKL typically in the the range 10^{-2} to 5×10^{-2} ppmV.

Cards 22-25 deal with species 3, aldehydes, KLMSOR=4, AMOL=38, PBGKL typically in the range 1×10^{-3} to 5×10^{-3} ppmV.

Cards 26-29 deal with species 4, nitrous acid, KLMSOR=0 (or 5), AMOL=47, PBGKL less than 10^{-3} ppmV, typically set to a very low value.

Cards 30-33 deal with species 5, nitric acid, KLMSOR=0 (or 5), AMOL=63, PBGKL less than 10^{-3} ppmV, typically set to a very low value.

```
ATTEMPT TO RUN STLOU DAY 195 1976 TRY 2
 LIRAQ 5 KM GRID     680.  780. 4220. 4320.
 06?00 DAY 195 1976  INITIAL TIME
 07?00 DAY 195 1976  FINAL TIME
 00?00               DAYLIGHT SAVING TIME SHIFT
 01?00               PRINT INTERVAL
 00?30               TIME HISTORY RECORD INTERVAL
 03?00               MASS BALANCE INTERVAL
 THE FOLLOWING STATIONS WILL HAVE TIME HISTORIES KEPT
   1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
  21  22  23  24  25   0
 THE FOLLOWING UTM LOCATIONS WILL HAVE TIME HISTORIES KEPT
   0
   1 ALKENES
 SOURCE COLUMN AND MULTIPLIERS                              3  1.0000E+00  1.0000E 00
 MOLECULAR WEIGHT     44.00
 BACKGROUND VALUES  W 2.001E-02 E 2.001E-02 S 2.001E-02 N 2.001E-02 A 2.001E-02
   2 ALKANES
 SOURCE COLUMN AND MULTIPLIERS                              2  1.0000E+00  1.0000E+00
 MOLECULAR WEIGHT     58.00
 BACKGROUND VALUE6  W 2.001E-02 E 2.001E-02 S 2.001E-02 N 2.001E-02 A 2.001E-02
   3 ALDEHYDES
 SOURCE COLUMN AND MULTIPLIERS                              4  1.0000E+00  1.0000E+00
 MOLECULAR WEIGHT     30.00
 BACKGROUND VALUES  W 4.001E-03 E 4.001E-03 S 4.001E-03 N 4.001E-03 A 4.001E-03
   4 NITROUS ACID
 SOURCE COLUMN AND MULTIPLIERS                              0  0.          0.
 MOLECULAR WEIGHT     47.00
 BACKGROUND VALUES  W 4.060E-08 E 4.060E-08 S 4.060E-08 N 4.060E-08 A 4.060E-08
   5 NITRIC ACID
 SOURCE COLUMN AND MULTIPLIERS                              0  0.          0.
 MOLECULAR WEIGHT     63.00
 BACKGROUND VALUES  W 4.060E-08 E 4.060E-08 S 4.060E-08 N 4.060E-08 A 4.060E-08
   6 HYDROGEN PEROXIDE
 SOURCE COLUMN AND MULTIPLIERS                              0  0.          0.
 MOLECULAR WEIGHT     34.00
 BACKGROUND VALUES  W 4.060E-08 E 4.060E-08 S 4.060E-08 N 4.060E-08 A 4.060E-08
   7 NITRIC OXIDE
 SOURCE COLUMN AND MULTIPLIERS                              5  0.9000E+00  0.9000E+00
 MOLECULAR WEIGHT     30.00
 BACKGROUND VALUES  W 1.001E-03 E 1.001E-03 S 1.001E-03 N 1.001E-03 A 1.001E-03
   8 NITROGEN DIOXIDE
 SOURCE COLUMN AND MULTIPLIERS                              5  0.1         0.1
 MOLECULAR WEIGHT     46.00
 BACKGROUND VALUES  W 1.001E-03 E 1.001E-03 S 1.001E-03 N 1.001E-03 A 1.001E-03
   9 OZONE
 SOURCE COLUMN AND MULTIPLIERS                              0  0.          0.
 MOLECULAR WEIGHT     48.00
 BACKGROUND VALUES  W 5.001E-02 E 5.001E-02 S 5.001E-02 N 5.001E-02 A 5.000E-02
  10 CARBON MONOXIDE
 SOURCE COLUMN AND MULTIPLIERS                              7  1.0000E+00  1.0000E+00
 MOLECULAR WEIGHT     28.00
 BACKGROUND VALUES  W 1.001E-01 E 1.001E-01 S 1.001E-01 N 1.001E-01 A 1.001E-01
  11 SULFUR DIOXIDE
 SOURCE COLUMN AND MULTIPLIERS                              6  1.0000E+00  1.0000E+00
 MOLECULAR WEIGHT     64.00
 BACKGROUND VALUES  W 1.001E-02 E 1.001E-02 S 1.001E-02 N 1.001E-02 A 1.001E-02
  12 SULFATE
 SOURCE COLUMN AND MULTIPLIERS                              0  0.          0.
 MOLECULAR WEIGHT    100.00
 BACKGROUND VALUES  W 1.001E-03 E 1.001E-03 S 1.001E-03 N 1.001E-03 A 1.001E-03


  0
1 1 1 0 0 0 1 1 1 1 1 0                POLLUTANT OUTPUT SELECTION
0
```

FIGURE H-1. Example of LIRAQ-2S QSRUN file.

Cards 34-37 deal with species 6, hydrogen peroxide, KLMSOR=0, AMOL=34, PBGKL less than 10^{-3} ppm V, typically set to a very low value.

Cards 38-41 deal with species 7, nitric oxide, KLMSOR=5, AMOL=30, PBGKL typically in the range 10^{-5} to 10^{-2} ppm V depending on area.

Cards 42-45 deal with species 8, nitrogen dioxide, KLMSOR=5 or 0, AMOL=46, PBGKL typically in the range 10^{-4} to 10^{-2} ppm V depending on area.

Cards 46-49 deal with species 9, ozone, KLMSOR=0, AMOL=48, PBGKL typically in the range 1-8 x 10^{-2} ppm V depending on area, day.

TABLE H-2. Formats of QSRUN data cards.

Card #	Columns	Format	Symbol	Units	Value limits	Typical value	Description
1	1-40	5A8	NAME	—	—	St. Louis day 195 1976 R2004	Problem name
2	1-18	6X,I2,10X	DX	km	1,2,3,4,5,...	5	Grid size
2	19-24	F6.0	UTME1	km	Within QGEO grid	680	UTM easting coordinate of west edge of domain
2	25-30	F6.0	UTME2	km	20DX greater than UTME1 and within QGEO	780	UTM easting coordinate of east edge of domain
2	31-36	F6.0	UTMN1	km	Within QGEO	4220	UTM northing coordinate of south edge of domain
2	37-42	F6.0	UTMN2	km	20DX greater than UTMN and within QGEO	4320	UTM northing coordinate of north edge of domain
3	1-19	2(1X,I2), 5X,I3,1X,I4	TIN	hr:min	Depends on meteorological data file	04:00 195 1976	Start time of model simulation
4	1-19	2(1X,I2), 5X,I3,1X,I4	TFIN	hr:min	Depends on meteorological data file	19:00 195 1976	Final time of model simulation
5	1-19	2(1X,I2), 5X,I3,1X,I4	TDS	hr:min	00:00 or 01:00	00:00	Daylight Savings Time shift
6	1-19	2(1X,I2), 5X,I3,1X,I4	TPINT	hr:min	00:30 to 03:00	01:00	Time interval between printed output of data

TABLE H-2. Continued.

Card #	Columns	Format	Symbol	Units	Value limits	Typical value	Description
7	1-19	2(1X,I2), 5X,I3,1X,I4	TRECI	hr:min	00:15 to 03:00	00:30	Time interval between keeping of data for station histories
8	1-19	2(1X,I2) 5X,I3,1X,I4	TIMBAL	hr:min	01:00 to 24:00	03:00	Time interval between mass balance calculations, not used in LIRAQ-2
9	—	—	—	—	—	—	Descriptive card
10,11	1-80	20I4	LOCHST	—	Station numbers identified on QGEO file	1	Stations numbers indicating stations at which to keep time histories
12	—	—	—	—	—	—	Descriptive card
13	1-80	10F8.0	LOCHST	Set of pairs of UTM coordinates	Within QGEO	690 4240	UTM location at which station history is to be kept
14	1-4	I4	NPL	—	1 to 12	1	Pollutant number
14	5-33	4A10	NTIT (NMPOL)	Hollerith	—	Alkenes	Pollutant name
15	51-54	50X,I4	KLMSOR	—	0, 1, 2, 3, 4, 5, 6, or 7	3	Column in QSOR file in which pollutant emissions to be found
15	55-78	2E12.4	SORMUL	—	None	1.0	Source multipliers to convert units or modify sources

TABLE H-2. Continued.

Card #	Columns	Format	Symbol	Units	Value limits	Typical value	Description
16	20-28	F8.0	AMOL	—	Depends on pollutant	28	Molecular weight of pollutant
17	29-79	5(2C,E10.3)	PBKGL	ppm	None, but must not create excessively sharp gradients	2.000E-2,2.000E-2 2.000E-2,2.000E-2 1.000E-2	Boundary concentration for pollutant on west, east, south, north, and above domain
18-61	Repeat of 14-17 for other pollutants						
62	1-4	I4	NPL	—	0	0	Terminates species data
63	1-30	15I2	MPLT	—	0 or 1	0	MLPT=1 species contours and station records are kept; MPLT=0 none are kept.
64	1-2	—	NEST	—	0 or 1	0	NEST=0 run is started from data on QICON. NEST=1 run is restarted from concentrations stored on QREST
65	1-5	I5	IS	—	1 to 15	1	Initial concentration of SPECIES. IS will be SCIN times the value from QREST
65	6-15	E10.2	SCIN	—	—	1.0E+00	
65	16-25	E10.2	SCUP	molecules/cm^3	—	0.00E+00 plus SCUP	
66	Same as 65					0	If no more data, IS=0

Cards 50-53 deal with carbon monoxide, KLMSOR=7, AMOL=28, PBGKL typically in the range 10^{-1} ppmV to 1. depending on area.

Cards 54-57 deal with sulfur dioxide, KLMSOR=6, AMOL=64, PBGKL typically in the range 10^{-3} to 10^{-2} ppmV depending on area.

Cards 58-61 deal with sulfate, KLMSOR=0, AMOL=98, PBGKL= whatever the data suggest.

Card 62 is a flag for end of data (0 in column 4).

Card 63 specifies the species for which records are to be kept in QSREC and graphical output. If VERF is to be used, only the three hydrocarbon species, NO, NO_2, O_3, CO, and SO_2 should have MPLT set equal to 1.

Card 64 specifies whether you wish to start the problem from QICON (NEST=0) or from a restart file (NEST=1). Starting from a restart tape can permit the user to continue a problem that aborted after finishing at least one edit. QREST stores the concentrations computed at the meteorological update periods. A restart from QREST is more likely to be useful in the context of running a single problem using several different projected emissions inventories such as might be carried out as part of a study designed to test control strategies than in verification runs. Starting from QREST can cut problem costs by ∿1000 computing units under some circumstances. This savings is worthwhile if a problem involves repeat runs with slight emissions modifications.

Cards 65 through the end permit the initial conditions to be scaled if and only if one is starting from QREST. This option is useful if one is running a day with projected future emissions inventories that differ from present inventories. This section must end with a card with blanks or zeros in columns 1-5.

QRAD

The file QRAD is a table of photodissociation rates as a function of the cosine of the solar zenith angle (Fig. H-2 and Table H-3). This file is generated by a special LLL program (QRADGEN), which carries out a calculation described in Appendix 5-3 of MacCracken (1975). The photodissociation rate coefficients for a purely absorbing atmosphere are evaluated for 50 equally spaced values, from 0.0 to 1.0, of the cosine of the zenith angle. A correction for scattering is then applied, and the coefficients are written into the data file QRAD. This file then provides the table of values used by PHODIS in the LIRAQ-2 calculation. The first card contains the increment of DCOS, the cosine of the zenith angle, and the remaining 50 lines contain a list of the

TABLE H-3. Format of QRAD data file.

Card No.	Columns	Format	Symbol	Units
1	1-12	E12.5	DCOS	—
2-51	13-120	9E12.5	QJT	s^{-1}

```
2.04082E-02                                          INCREMENT IN THE COS OF THE ZENITH ANGLE
1.00000E+00 1.18952E-02 2.19282E-03 5.52738E-06 2.71285E-05 1.91250E-03 2.71285E-05 2.88974E-03 5.17648E-04 2.230  E-05
9.79592E-01 1.17920E-02 2.16940E-03 5.34053E-06 2.65965E-05 1.90391E-03 2.65965E-05 2.87616E-03 5.12557E-04 2.11081E-05
9.59184E-01 1.16888E-02 2.14597E-03 5.15563E-06 2.60658E-05 1.89533E-03 2.60658E-05 2.86253E-03 5.07454E-04 1.99530E-05
9.38776E-01 1.15641E-02 2.12253E-03 4.96726E-06 2.55107E-05 1.88373E-03 2.55107E-05 2.84731E-03 5.02340E-04 1.87948E-05
9.18367E-01 1.14219E-02 2.09907E-03 4.77674E-06 2.49363E-05 1.86968E-03 2.49363E-05 2.83076E-03 4.97212E-04 1.76457E-05
8.97959E-01 1.12816E-02 2.07531E-03 4.58868E-06 2.43648E-05 1.85516E-03 2.43648E-05 2.81417E-03 4.92072E-04 1.65414E-05
8.77551E-01 1.11587E-02 2.04893E-03 4.40312E-06 2.38038E-05 1.83643E-03 2.38038E-05 2.79752E-03 4.86918E-04 1.54813E-05
8.57143E-01 1.10356E-02 2.02253E-03 4.22011E-06 2.32448E-05 1.81769E-03 2.32448E-05 2.78081E-03 4.81750E-04 1.44648E-05
8.36735E-01 1.09000E-02 1.99517E-03 4.03393E-06 2.26523E-05 1.80099E-03 2.26523E-05 2.76221E-03 4.76567E-04 1.35114E-05
8.16327E-01 1.07574E-02 1.96730E-03 3.84763E-06 2.20436E-05 1.78538E-03 2.20436E-05 2.74257E-03 4.71368E-04 1.26086E-05
7.95918E-01 1.06071E-02 1.93868E-03 3.66279E-06 2.14359E-05 1.76571E-03 2.14359E-05 2.72323E-03 4.66153E-04 1.17339E-05
7.75510E-01 1.04259E-02 1.90716E-03 3.47466E-06 2.08243E-05 1.72980E-03 2.08243E-05 2.70532E-03 4.60920E-04 1.08864E-05
7.55102E-01 1.02446E-02 1.87563E-03 3.29025E-06 2.02158E-05 1.69389E-03 2.02158E-05 2.68732E-03 4.55670E-04 1.00740E-05
7.34694E-01 1.00344E-02 1.84083E-03 3.11198E-06 1.95779E-05 1.65857E-03 1.95779E-05 2.66714E-03 4.50400E-04 9.31899E-06
7.14286E-01 9.81460E-03 1.80494E-03 2.93822E-06 1.89331E-05 1.62344E-03 1.89331E-05 2.64616E-03 4.45109E-04 8.60636E-06
6.93878E-01 9.59481E-03 1.76860E-03 2.76692E-06 1.82925E-05 1.58761E-03 1.82925E-05 2.62480E-03 4.39552E-04 7.91618E-06
6.73469E-01 9.37504E-03 1.73125E-03 2.59661E-06 1.76563E-05 1.55014E-03 1.76563E-05 2.60269E-03 4.33404E-04 7.23385E-06
6.53061E-01 9.15530E-03 1.69389E-03 2.43055E-06 1.70245E-05 1.51267E-03 1.70245E-05 2.58046E-03 4.27239E-04 6.59027E-06
6.32653E-01 8.91927E-03 1.64978E-03 2.26661E-06 1.63617E-05 1.47188E-03 1.63617E-05 2.55731E-03 4.21056E-04 5.99965E-06
6.12245E-01 8.68041E-03 1.60449E-03 2.10691E-06 1.56981E-05 1.43051E-03 1.56981E-05 2.53389E-03 4.14854E-04 5.44647E-06
5.91837E-01 8.41865E-03 1.55891E-03 1.95100E-06 1.50401E-05 1.38758E-03 1.50401E-05 2.50920E-03 4.08311E-04 4.92080E-06
5.71429E-01 8.12258E-03 1.51291E-03 1.79867E-06 1.43880E-05 1.34230E-03 1.43880E-05 2.48268E-03 4.01272E-04 4.42016E-06
5.51020E-01 7.82670E-03 1.46690E-03 1.65155E-06 1.37417E-05 1.29703E-03 1.37417E-05 2.45599E-03 3.94216E-04 3.95356E-06
5.30612E-01 7.56726E-03 1.42022E-03 1.51485E-06 1.30415E-05 1.24730E-03 1.30415E-05 2.42559E-03 3.87140E-04 3.51998E-06
5.10204E-01 7.30983E-03 1.37352E-03 1.38338E-06 1.23459E-05 1.19734E-03 1.23459E-05 2.39480E-03 3.80043E-04 3.11837E-06
4.89796E-01 7.04300E-03 1.32288E-03 1.25221E-06 1.16623E-05 1.14348E-03 1.16623E-05 2.36240E-03 3.72919E-04 2.74768E-06
4.69388E-01 6.76683E-03 1.26833E-03 1.12228E-06 1.09906E-05 1.08571E-03 1.09906E-05 2.32836E-03 3.65766E-04 2.40685E-06
4.48980E-01 6.48893E-03 1.21376E-03 9.98859E-07 1.03254E-05 1.02791E-03 1.03254E-05 2.29363E-03 3.58578E-04 2.09476E-06
4.28571E-01 6.17527E-03 1.15855E-03 8.82808E-07 9.63391E-06 9.69364E-04 9.63391E-06 2.25076E-03 3.51350E-04 1.81031E-06
4.08163E-01 5.86193E-03 1.10337E-03 7.73433E-07 8.95258E-06 9.10818E-04 8.95258E-06 2.20756E-03 3.44075E-04 1.55236E-06
3.87755E-01 5.57158E-03 1.04439E-03 6.72130E-07 8.27753E-06 8.54146E-04 8.27753E-06 2.15962E-03 3.35849E-04 1.31591E-06
3.67347E-01 5.29659E-03 9.82917E-04 5.78380E-07 7.61087E-06 7.98722E-04 7.61087E-06 2.10836E-03 3.26982E-04 1.10221E-06
3.46939E-01 5.01338E-03 9.21192E-04 4.91793E-07 6.95401E-06 7.43299E-04 6.95401E-06 2.05529E-03 3.18172E-04 9.13541E-07
3.26531E-01 4.68270E-03 8.57742E-04 4.13869E-07 6.29837E-06 6.87876E-04 6.29837E-06 1.99404E-03 3.09910E-04 7.51342E-07
3.06122E-01 4.35259E-03 7.94388E-04 3.42605E-07 5.65665E-06 6.32452E-04 5.65665E-06 1.93223E-03 3.01548E-04 6.09534E-07
2.85714E-01 4.03616E-03 7.27212E-04 2.76419E-07 5.02540E-06 5.79214E-04 5.02540E-06 1.86600E-03 2.92567E-04 4.82263E-07
2.65306E-01 3.72592E-03 6.58506E-04 2.16953E-07 4.40872E-06 5.26913E-04 4.40872E-06 1.79739E-03 2.83233E-04 3.72521E-07
2.44898E-01 3.41172E-03 5.89107E-04 1.65328E-07 3.80570E-06 4.75588E-04 3.80570E-06 1.72565E-03 2.73204E-04 2.82138E-07
2.24490E-01 3.08446E-03 5.17329E-04 1.21812E-07 3.21024E-06 4.27190E-04 3.21024E-06 1.64621E-03 2.61434E-04 2.10742E-07
2.04082E-01 2.75823E-03 4.45836E-04 8.55645E-08 2.63897E-06 3.78792E-04 2.63897E-06 1.56543E-03 2.49433E-04 1.52763E-07
1.83673E-01 2.46236E-03 3.79647E-04 5.71834E-08 2.15378E-06 3.32892E-04 2.15378E-06 1.46648E-03 2.35548E-04 1.07719E-07
1.63265E-01 2.17478E-03 3.15060E-04 3.53897E-08 1.70781E-06 2.87617E-04 1.70781E-06 1.36162E-03 2.20910E-04 7.29258E-08
1.42857E-01 1.88831E-03 2.55917E-04 1.98131E-08 1.30920E-06 2.44254E-04 1.30920E-06 1.24504E-03 2.04888E-04 4.67526E-08
1.22449E-01 1.60319E-03 2.06450E-04 9.70144E-09 9.73749E-07 2.04442E-04 9.73749E-07 1.10861E-03 1.86599E-04 2.78861E-08
1.02041E-01 1.31975E-03 1.57451E-04 3.73432E-09 6.69055E-07 1.64631E-04 6.69055E-07 9.68660E-04 1.67327E-04 1.50454E-08
8.16327E-02 1.03845E-03 1.18515E-04 9.93402E-10 4.37171E-07 1.29738E-04 4.37171E-07 7.90341E-04 1.39757E-04 7.00661E-09
6.12245E-02 7.60084E-04 8.11869E-05 1.21079E-10 2.44942E-07 9.53908E-05 2.44942E-07 6.03789E-04 1.09930E-04 2.59353E-09
4.08163E-02 4.86057E-04 4.86444E-05 2.28252E-12 1.07792E-07 6.24490E-05 1.07792E-07 3.71632E-04 6.73393E-05 6.37347E-10
2.04082E-02 2.19772E-04 2.18154E-05 3.03908E-17 2.87893E-08 3.12245E-05 2.87893E-08 1.18202E-04 1.92930E-05 5.54079E-11
0.          0.          0.          0.          0.          0.          0.          0.          0.          0.
```

FIGURE H-2. Example of a QRAD file.

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD, BEGIN SECTION HERE
BEGIN LAST LINE OF TEXT
3/8"
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
PAGE NUMBER
EPA-287 (Cin.)
(4-79)

cosine of the zenith angle and the 9 photodissociation rate coefficients appropriate for that angle. The subroutine PHODIS then performs a table lookup from this list.

QREST

The file QREST is a binary file that is both a receiver of data and a potential input file. Vertical average concentrations in molecules/cm^3 are written to the file at the time of each call to YOUT and at the beginning and end of each model run. If a terminated problem is to be run (with possible modifications), QREST may be used to provide the initial conditions. The first 97 words on this file are reserved for a record of those times at which concentrations have been written on it. The remainder of the space is available for storing concentrations of all species at all grid points at the times recorded. When a problem is restarted at time TIN, the variable TP(100) is set, and the RESTART subroutine determines where on QREST the concentrations corresponding to that time are stored, buffers them in, and scales them as described in the discussion of the restart portion of QSRUN.

LIRAQ-2S OUTPUT FILES

LIRAQ-2S output files are listed in Table H-4. The files OUTPUT, QSREC, and QGRAPH are essentially the same for LIRAQ-2S as for LIRAQ-1S, except that more species may be examined in LIRAQ-2S. Sample QGRAPH output is given in Fig. H-3.

QHSP

QHSP files generated by LIRAQ-2S will be much more extensive than those generated by LIRAQ-1S, because they include more species and because computed reaction rates are output as are boundary conditions, unlike LIRAQ-1S, LIRAQ-2S does not output mass balance tabulations or mass fluxes. Sample LIRAQ-2S tabular output is given in Fig. H-4.

TABLE H-4. LIRAQ-2S output files.

File	Content	Use	Where described
OUTPUT	Diagnostic error messages	Diagnostic	LBL User's Manual
QSTEP	LIRAQ-2S time steps	Diagnostic	Below
QSREC	Computed concentrations at selected stations as a function of time	Verification	Appendix G
QHSP	Tabular output	Interpretation of air quality	Appendix G
QGRAPH	Graphical output	Interpretation of air quality	Appendix G
QREST	Restart data	To restart problem	Above

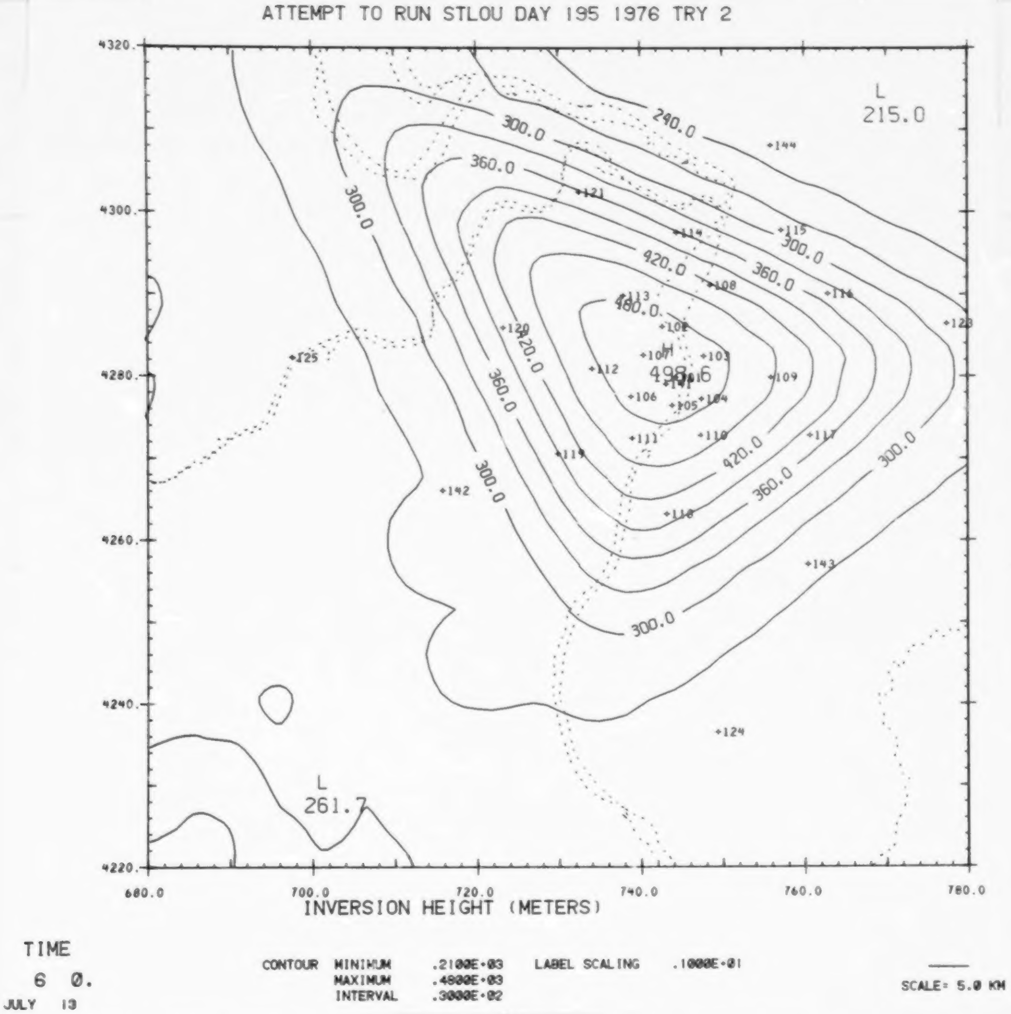

FIGURE H-3a. QGRAPH presents a graphical display of inversion height and pollutant concentrations, both as computed 1 meter above the surface and averaged over the mean layer. These plots are contour diagrams superimposed on a map. It also contains a plot of pollutant concentration vs. time for the stations selected in QSRUN.

QSTEP

QSTEP contains LIRAQ-2S timesteps and some additional diagnostic messages. In LIRAQ-2S there is no Courant condition, and the time steps reflect the lesser of 900 seconds or a time step determined by the time constants for the evolution of the photochemical system. In a normal run, these timesteps will be very small whenever a discontinuous change is imposed on the system (e.g., initiation, sunrise, sunset, meteorological updates). If the problem is running normally there will be an irregular, but nearly monotonic increase from time steps of $\sim 10^{-3}$ seconds up to time steps of

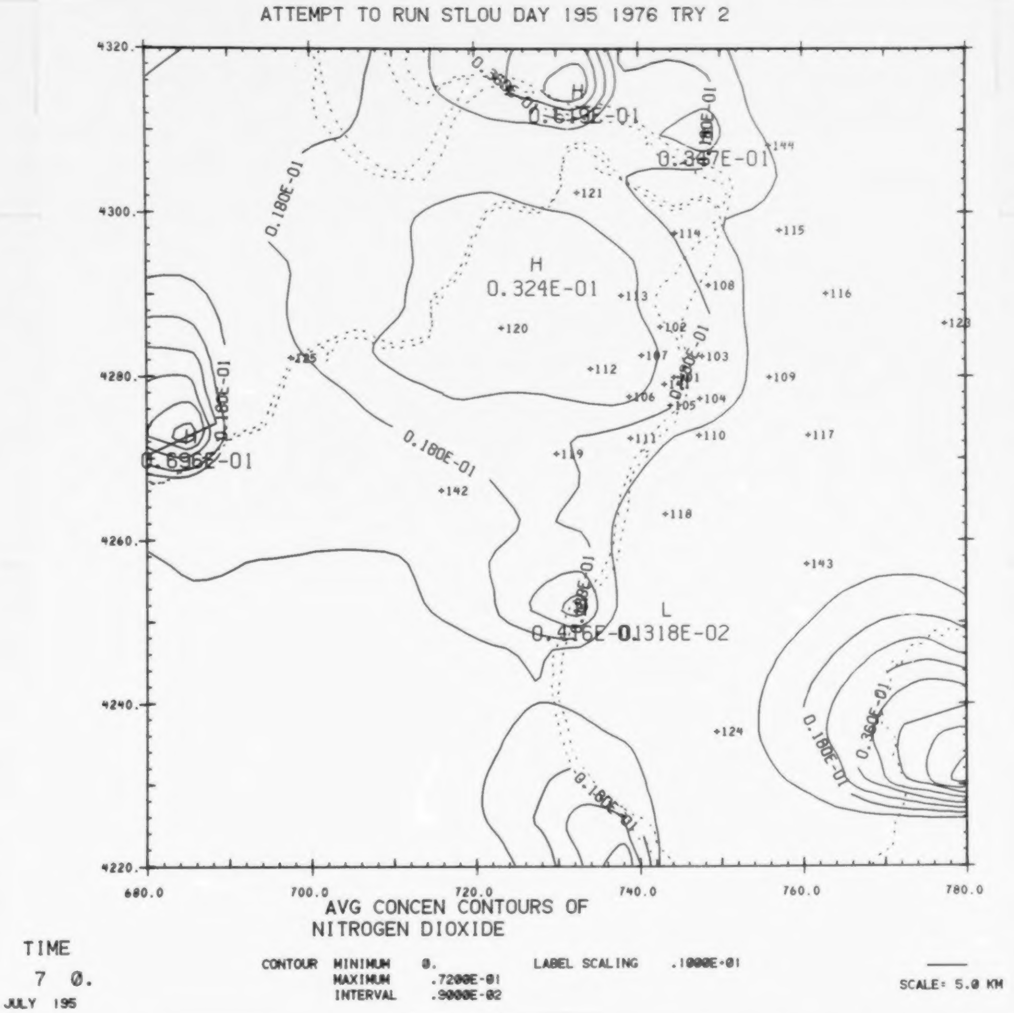

FIGURE H-3b. Continued. Similar to H-3a except contours give concentrations of NO_2 averaged over the mixed layer. Similar plots are produced for all pollutants selected for graphical display in the QSRUN file.

several hundred seconds. Under some circumstances (e.g., at night, if some portions of the grid contain more NO than O_3 and other portions contain more O_3 than NO) the time steps will remain small and the problem will consume a large amount of computer time. Also, if the problem attempts to compute a negative concentration at any point, the time step will be decreased and all negative concentrations computed in the unsuccessful attempted timestep will be reported in QSTEP. In practice, LIRAQ will never accept a time step that leads to negative concentrations. But on a failed time step, negative concentrations indicate that the code is having difficulty in integrating to a solution. Usually this reflects the rapid decay of a species without a chemical source (e.g., O_3 or occasionally NO at night) the correct solution under those circumstances will usually be a near zero concentration. Although rapidly

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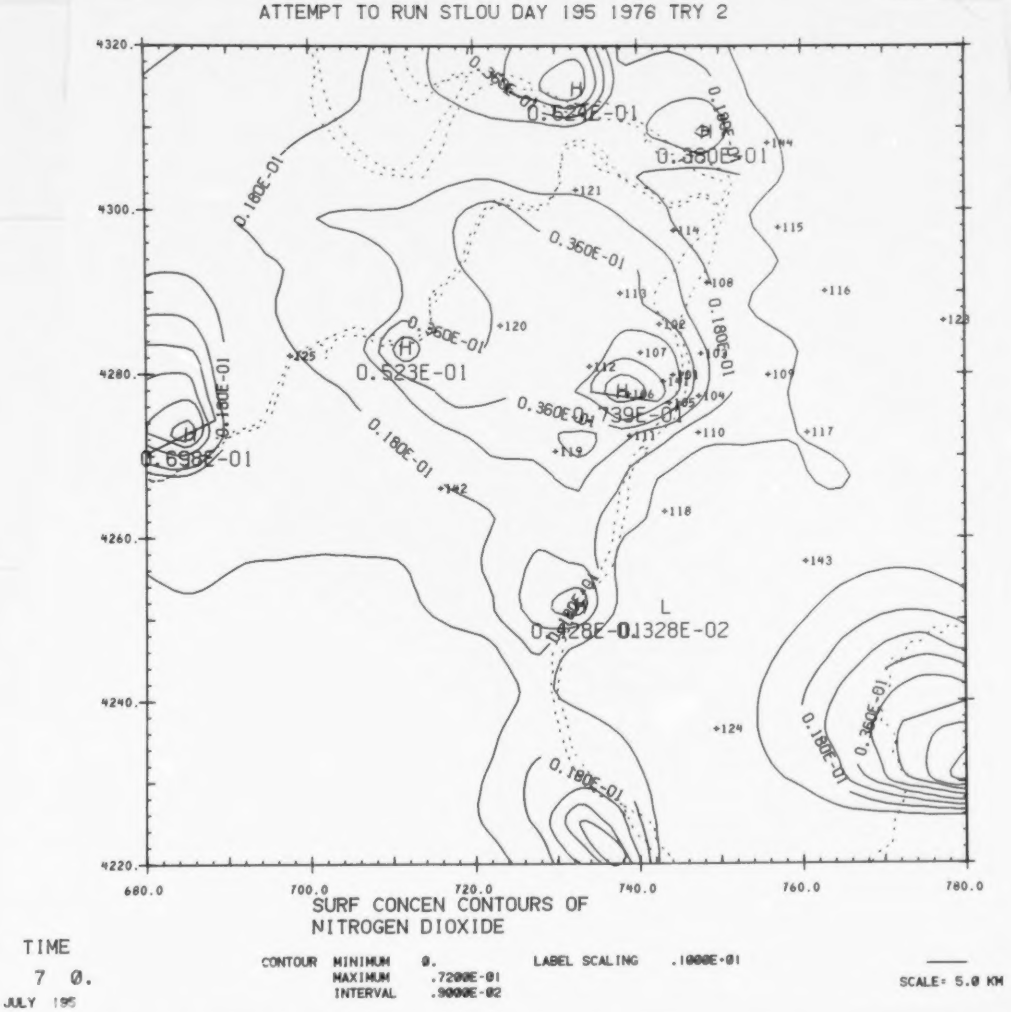

FIGURE H-3c. Continued. Similar to H-3b except concentrations are computed for 1 m above the surface.

decaying nighttime ozone or NO will usually be the cause of any negative concentrations, if any species is computed to have even very small negative concentrations, other species may have gross errors, and may even go negative.

If LIRAQ-2S maintains a very small time step or displays more than a very few episodes of negative computed concentrations, it may be desirable to carefully examine the input and avoid the time or locations responsible for the computational problems. Figure H-5 gives a sample QSTEP file.

Control Card Deck

The control card decks are discussed in Appendix J.

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BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/16"
PAGE NUMBER
EPA-287 (Cin.) 10-76

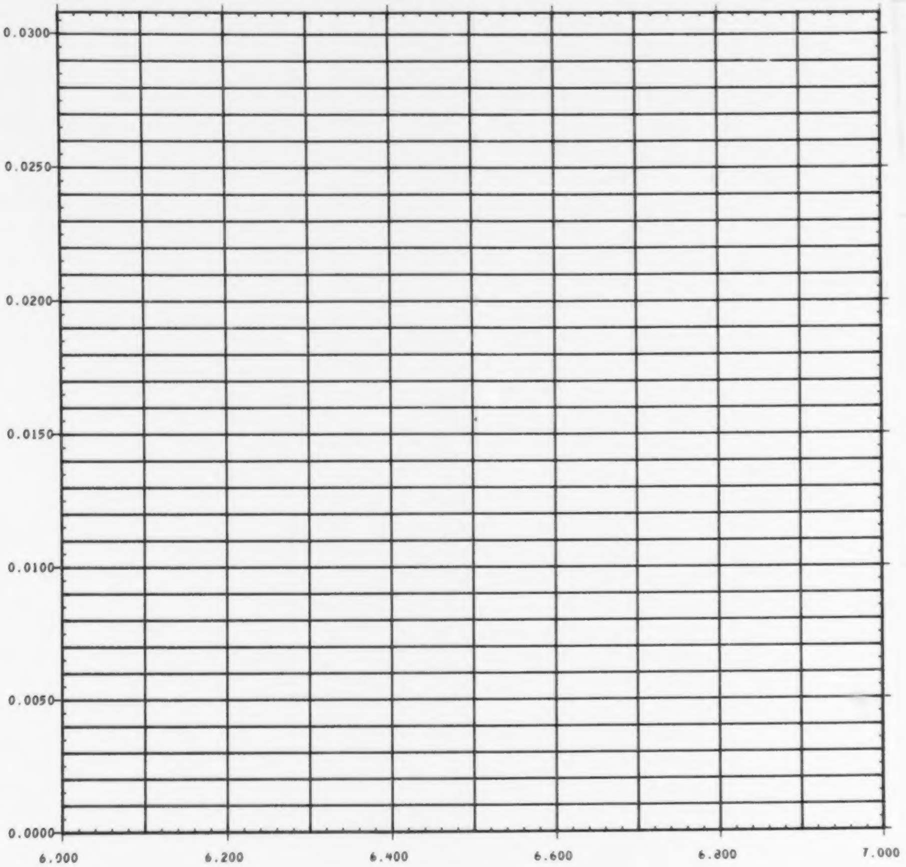


FIGURE H-3d. Continued. Grid used to report alkene concentrations vs. model time. Similar plots are provided for all pollutants selected in the QSRUN file.

DAYFILE

The LBL system generated file DAYFILE for a LIRAQ-2S run will include the central processor time used between calls to YOUT. This is useful in analyzing problems that consume an excessive amount of computer time.

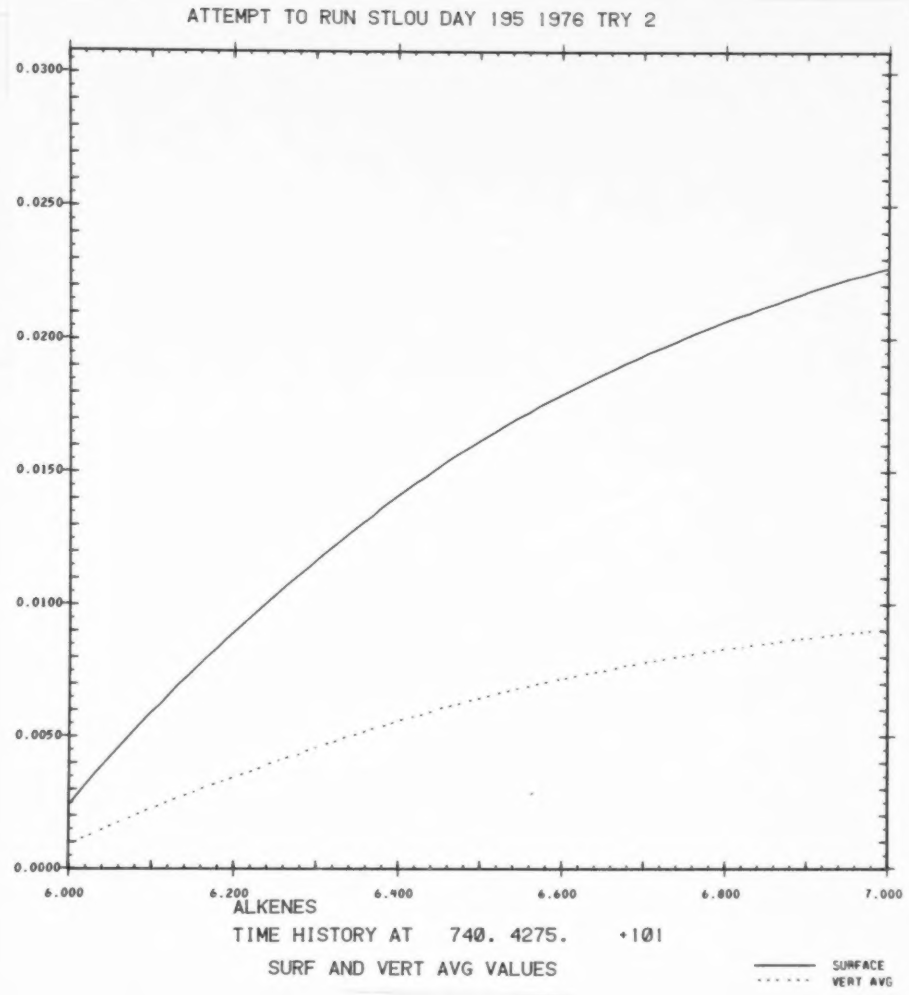
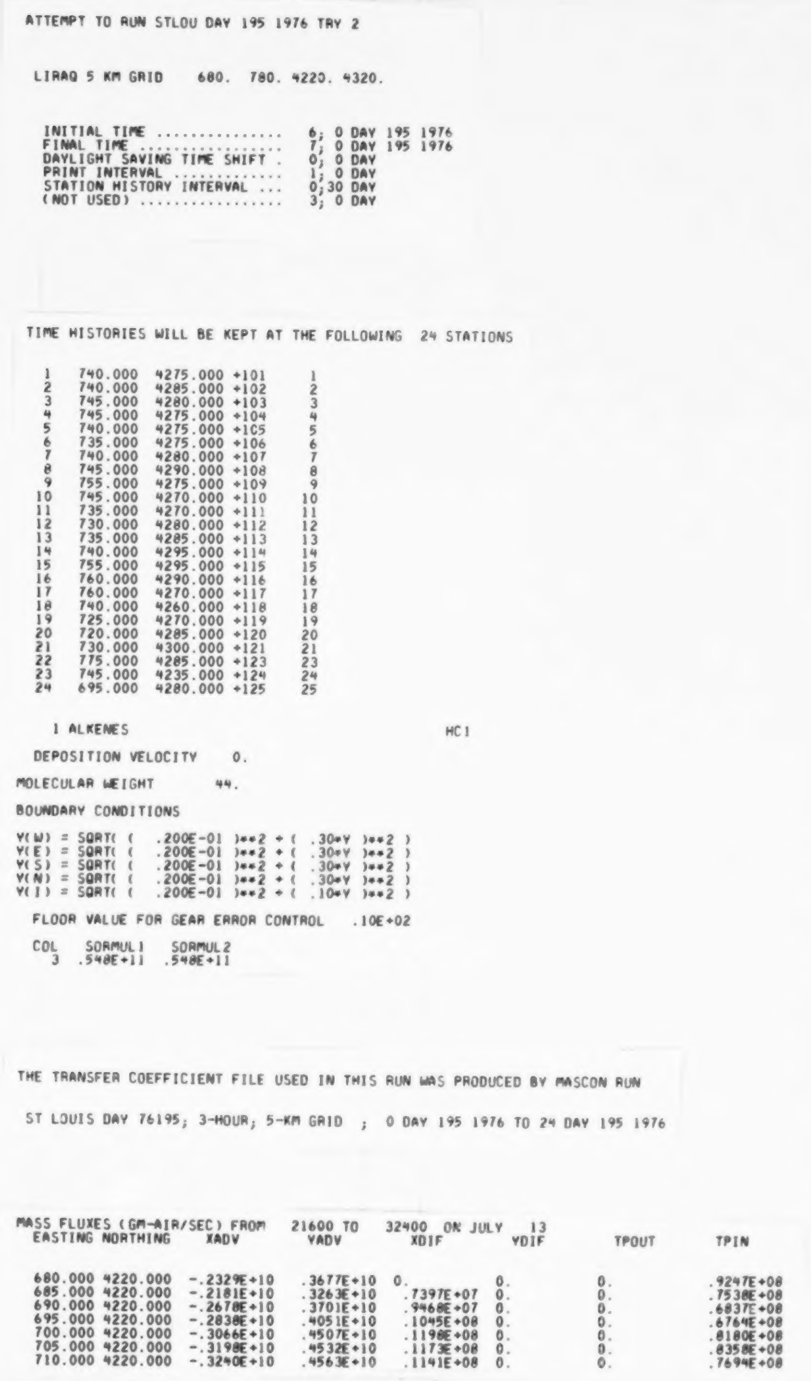


FIGURE H-3e. Continued. Computed concentrations of alkenes vs. time at station 101. Similar plots are produced for all pollutants and locations requested in the QSRUN file.



```
ATTEMPT TO RUN STLOU DAY 195 1976 TRY 2


 LIRAQ 5 KM GRID    680.  780. 4220. 4320.


  INITIAL TIME ...............   6; 0 DAY 195 1976
  FINAL TIME .................   7; 0 DAY 195 1976
  DAYLIGHT SAVING TIME SHIFT .   0; 0 DAY
  PRINT INTERVAL .............   1; 0 DAY
  STATION HISTORY INTERVAL ...   0;30 DAY
  (NOT USED) .................   3; 0 DAY
```

```
TIME HISTORIES WILL BE KEPT AT THE FOLLOWING  24 STATIONS

   1    740.000  4275.000 +101      1
   2    740.000  4285.000 +102      2
   3    745.000  4280.000 +103      3
   4    745.000  4275.000 +104      4
   5    740.000  4275.000 +1C5      5
   6    735.000  4275.000 +106      6
   7    740.000  4280.000 +107      7
   8    745.000  4290.000 +108      8
   9    755.000  4275.000 +109      9
  10    745.000  4270.000 +110     10
  11    735.000  4270.000 +111     11
  12    730.000  4280.000 +112     12
  13    735.000  4285.000 +113     13
  14    740.000  4295.000 +114     14
  15    755.000  4295.000 +115     15
  16    760.000  4290.000 +116     16
  17    760.000  4270.000 +117     17
  18    740.000  4260.000 +118     18
  19    725.000  4270.000 +119     19
  20    720.000  4285.000 +120     20
  21    730.000  4300.000 +121     21
  22    775.000  4285.000 +123     23
  23    745.000  4235.000 +124     24
  24    695.000  4280.000 +125     25

   1 ALKENES                                     HC1

  DEPOSITION VELOCITY    0.

MOLECULAR WEIGHT       44.

BOUNDARY CONDITIONS

Y(W) = SQRT( (   .200E-01 )**2 + (  .30*Y  )**2 )
Y(E) = SQRT( (   .200E-01 )**2 + (  .30*Y  )**2 )
Y(S) = SQRT( (   .200E-01 )**2 + (  .30*Y  )**2 )
Y(N) = SQRT( (   .200E-01 )**2 + (  .30*Y  )**2 )
Y(I) = SQRT( (   .200E-01 )**2 + (  .10*Y  )**2 )

  FLOOR VALUE FOR GEAR ERROR CONTROL   .10E+02

  COL   SORMUL1   SORMUL2
    3  .548E+11  .548E+11
```

```
THE TRANSFER COEFFICIENT FILE USED IN THIS RUN WAS PRODUCED BY MASCON RUN

 ST LOUIS DAY 76195; 3-HOUR; 5-KM GRID  ;  0 DAY 195 1976 TO 24 DAY 195 1976
```

```
MASS FLUXES (GM-AIR/SEC) FROM    21600 TO    32400  ON JULY   13
  EASTING NORTHING     XADV         YADV         XDIF          YDIF          TPOUT         TPIN

  680.000 4220.000  -.2329E+10   .3677E+10  0.             0.            0.            .9247E+08
  685.000 4220.000  -.2181E+10   .3263E+10   .7397E+07  0.            0.            .7538E+08
  690.000 4220.000  -.2678E+10   .3701E+10   .9468E+07  0.            0.            .6837E+08
  695.000 4220.000  -.2838E+10   .4051E+10   .1045E+08  0.            0.            .6764E+08
  700.000 4220.000  -.3066E+10   .4507E+10   .1198E+08  0.            0.            .8180E+08
  705.000 4220.000  -.3198E+10   .4532E+10   .1173E+08  0.            0.            .8358E+08
  710.000 4220.000  -.3240E+10   .4563E+10   .1141E+08  0.            0.            .7694E+08
```

FIGURE H-4. Sample LIRAQ-2S QHSP output.

```
INVERSION HEIGHT ABOVE TOPO (M)
THE TIME IS NOW    6.00000 HOURS

  680.000 4315.000  .204E+03  .194E+03  .207E+03  .234E+03  .220E+03  .217E+03  .212E+03  .178E+03  .180E+03  .176E+03
  730.000 4315.000  .176E+03  .186E+03  .169E+03  .165E+03  .177E+03  .171E+03  .164E+03  .170E+03  .174E+03  .165E+03

  680.000 4310.000  .212E+03  .208E+03  .217E+03  .239E+03  .244E+03  .244E+03  .254E+03  .256E+03  .249E+03  .226E+03
  730.000 4310.000  .213E+03  .213E+03  .191E+03  .186E+03  .191E+03  .182E+03  .176E+03  .179E+03  .177E+03  .171E+03

  680.000 4305.000  .212E+03  .216E+03  .218E+03  .232E+03  .252E+03  .263E+03  .281E+03  .290E+03  .281E+03  .269E+03
  730.000 4305.000  .249E+03  .237E+03  .225E+03  .214E+03  .206E+03  .196E+03  .189E+03  .184E+03  .182E+03  .179E+03

  680.000 4300.000  .198E+03  .201E+03  .207E+03  .223E+03  .245E+03  .271E+03  .297E+03  .317E+03  .321E+03  .303E+03
  730.000 4300.000  .275E+03  .261E+03  .252E+03  .245E+03  .231E+03  .212E+03  .198E+03  .187E+03  .185E+03  .184E+03

  680.000 4295.000  .176E+03  .185E+03  .194E+03  .204E+03  .226E+03  .253E+03  .274E+03  .313E+03  .341E+03  .330E+03
  730.000 4295.000  .308E+03  .295E+03  .289E+03  .281E+03  .263E+03  .237E+03  .210E+03  .191E+03  .189E+03  .192E+03

  680.000 4290.000  .158E+03  .183E+03  .194E+03  .200E+03  .215E+03  .226E+03  .249E+03  .299E+03  .328E+03  .335E+03
  730.000 4290.000  .339E+03  .338E+03  .343E+03  .334E+03  .309E+03  .278E+03  .239E+03  .209E+03  .203E+03  .206E+03

  680.000 4285.000  .144E+03  .165E+03  .176E+03  .189E+03  .212E+03  .225E+03  .248E+03  .283E+03  .301E+03  .320E+03
  730.000 4285.000  .349E+03  .369E+03  .385E+03  .383E+03  .359E+03  .323E+03  .279E+03  .242E+03  .228E+03  .224E+03
```

```
 H2O (NO./CM3)    .2940E+18

  EACTION RATE COEFFICIENTS

       Q(  1) =      .146E-13
       Q(  2) =      .178E-13
       Q(  3) =      .231E-11
       Q(  4) =      .910E-11
       Q(  5) =      .236E-11
       Q(  6) =      .296E-16
       Q(  7) =      .380E-11
       Q(  8) =      .203E+00
       Q(  9) =      .870E-11
       Q( 10) =      .465E-20
       Q( 11) =      .100E-10
       Q( 12) =      .600E-11
       Q( 13) =      .140E-12
       Q( 14) =      .309E-11
       Q( 15) =      .299E-11
       Q( 16) =      .119E-16
       Q( 17) =      .267E-10
       Q( 18) =      .389E-13
       Q( 19) =      .220E-11
       Q( 20) =      .463E-11
       Q( 21) =      .146E-11
       Q( 22) =      .110E-11
       Q( 23) =      .270E-12
       Q( 24) =      .622E-15
       Q( 25) =      .200E-11
       Q( 26) =      .200E-11
       Q( 27) =      .318E-11
       Q( 28) =      .270E-11
       Q( 29) =      .270E-12
       Q( 30) =      .156E-12
       Q( 31) =      .324E-17
       Q( 32) =      .274E-17
       Q( 33) =      .500E-17
       Q( 34) =      .178E-13
       Q( 35) =      .146E-15
       Q( 36) =      .200E-10
       Q( 37) =      .927E-11
       Q( 38) =      .100E-14
       Q( 39) =      .927E-11
       Q( 40) =      .900E-13
       Q( 41) =      .600E-12
       Q( 42) =      .400E-12
       Q( 43) =      .200E-17
       Q( 44) =      .558E-13
       Q( 45) =      .100E-11
       Q( 46) =      .456E-14
       Q( 47) =      .449E-16
       Q( 48) =      .100E-18
INITIAL MET READ AT  21600 NEXT READ AT  32400
```

FIGURE H-4. Continued.

```
     SOURCES FROM    6 TO    7 ON 195/1976

ELEVATED SOURCES

                HC2          HC1          HC4          NO           SO2          CO
 735 4220   .1877E+01    .4357E+00    .3304E+00    .6037E+03    .2294E+04    .2012E+02
 730 4225   0.           0.           0.           .4488E+02    .4108E+03    0.
 725 4230   .7058E-02    .1639E-02    .1241E-02    .4539E+01    .4444E-02    .1286E+00
 775 4230   .6527E+01    .1515E+01    .1149E+01    .3068E+04    .7499E+04    .6998E+02
 725 4235   0.           0.           0.           0.           .9339E+03    0.
 730 4250   .1936E+01    .4493E+00    .3407E+00    .6226E+03    .2705E+04    .2076E+02
 735 4260   .7466E-02    .1739E-02    .1317E-02    .3600E+00    .2500E-02    .6000E-01
 775 4260   .3869E-01    .8985E-02    .6815E-02    .3111E+01    .1444E+02    .3044E+00
 720 4265   .6954E-02    .1604E-02    .1216E-02    .4488E+01    .4444E-02    .1272E+00
 730 4265   0.           0.           0.           .3188E+02    .1145E+03    0.
 735 4265   .1808E+01    .1367E+01    .4768E-01    .3171E+02    .1844E+03    .2218E+01
 760 4265   .4405E-01    .1022E-01    .7752E-02    .2209E+01    .5752E+01    .2725E+00
 685 4270   .8591E+01    .1994E+01    .1512E+01    .2763E+04    .1110E+05    .9211E+02
 740 4270   .8332E+00    .6888E+00    .1158E+00    .3721E+01    .4651E+01    .6511E+02
 735 4275   .5038E-01    .1169E-01    .8867E-02    .2431E+01    .1481E+02    .2120E+02
 740 4275   .4125E+02    .3116E+02    .4386E-01    .3949E+02    .7561E+02    .8940E+03
 745 4275   .4486E+00    .1041E+00    .7895E-01    .4715E+02    .1653E+03    .3406E+01
 730 4280   .3801E-01    .8820E-02    .6688E-02    .1834E+01    .9133E+01    .2703E+00
 735 4280   .1263E+00    .2932E-01    .2223E-01    .6093E+01    .5356E+02    .8125E+00
 740 4280   .9665E+00    .7198E+00    .1393E+00    .2077E+02    .5003E+02    .6624E+02
 745 4280   .8477E+00    .1968E+00    .1492E+00    .1636E+03    .3713E+03    .8682E+01
 735 4285   0.           0.           0.           0.           0.           .3963E+02
 745 4285   .9666E+01    .7563E+01    .4484E-02    .9557E+02    .2133E+03    .1105E+04
 725 4290   .7553E-02    .1745E-02    .1317E-02    .1866E+01    .4444E-02    .1378E+00
 730 4290   .6299E-02    .1474E-02    .1115E-02    .1548E+01    .3889E-02    .1142E+00
 740 4290   0.           0.           0.           .7008E+02    .2666E+02    0.
 750 4300   .6999E+02    .1205E+02    .3910E+00    .1160E+03    .1752E+04    .1915E+04
 755 4300   0.           0.           0.           0.           .1575E+02    0.
 740 4305   .7105E-03    .1650E-03    .1267E-03    .4583E-01    .1611E-01    .3056E-02
 745 4305   .2106E+01    .4889E+00    .3707E+00    .4348E+03    .1652E+04    .2244E+02
 730 4310   .3405E+01    .7903E+00    .5993E+00    .2008E+04    .4217E+04    .3651E+02

URFACE SOURCES

               HC2          HC1          HC4          NO           SO2          CO
 680 4230   .4883E-01    .2173E-01    .1178E-01    .4917E+00    .3611E-01    .1894E+01
 680 4235   .6200E+00    .3307E+00    .7397E-01    .1180E+01    .6944E-01    .1274E+02
 680 4240   .6200E+00    .3307E+00    .7397E-01    .1180E+01    .6944E-01    .1274E+02
 680 4245   .9772E+00    .4865E+00    .1091E+00    .2416E+01    .1306E+00    .1515E+02
 680 4250   .9772E+00    .4865E+00    .1091E+00    .2416E+01    .1306E+00    .1515E+02
 680 4255   .4346E+01    .2216E+01    .4543E+00    .7882E+01    .3424E+00    .7093E+02
 680 4260   .4346E+01    .2216E+01    .4543E+00    .7882E+01    .3424E+00    .7093E+02
 680 4265   .1085E+01    .6090E+00    .1730E+00    .2889E+01    .2694E+00    .2333E+02
 680 4270   .1208E+01    .3936E+00    .4446E-01    .7500E+00    .5278E-01    .7817E+01


 775 4270   .1846E+01    .6641E+00    .1159E+00    .2925E+01    .2000E+00    .1887E+02
 775 4275   .4257E+01    .1881E+01    .3434E+00    .5586E+01    .3583E+00    .5730E+02
 775 4280   .8483E+00    .4548E+00    .1159E+00    .2872E+01    .1944E+00    .1895E+02
 775 4285   .1635E+01    .8257E+00    .1918E+00    .4670E+01    .2903E+00    .2959E+02
 775 4290   .1635E+01    .8257E+00    .1918E+00    .4670E+01    .2903E+00    .2959E+02
 775 4295   .1861E+01    .9030E+00    .1956E+00    .4477E+01    .2479E+00    .3087E+02
 775 4300   .1861E+01    .9030E+00    .1956E+00    .4477E+01    .2479E+00    .3087E+02
 775 4305   .1899E+01    .9920E+00    .2298E+00    .4834E+01    .2785E+00    .3665E+02
 775 4310   .1899E+01    .9920E+00    .2298E+00    .4834E+01    .2785E+00    .3665E+02
 775 4315   .3475E+01    .1830E+01    .4284E+00    .8981E+01    .5667E+00    .5828E+02
INITIAL SOURCE READ AT  21600 NEXT READ AT  23400


 THE GAUSSIAN INTERPOLATION CONSTANT IS    .1000E+00
 AT LEAST  3 DATA POINTS WILL BE SOUGHT WITHIN A RADIUS OF  20 GRID ELEMENTS


 REFERENCE HEIGHT OF OBSERVATIONS (CM)    .1000E+03
```

FIGURE H-4. Continued.

```
POLLUTANT  NITROGEN DIOXIDE
SOURCE COLUMN  5
MOLECULAR WEIGHT     46.00
BACKGROUND VALUES]  WEST     .1001E-02 EAST     .1001E-02
  SOUTH    .1001E-02 NORTH    .1001E-02 TOP      .1001E-02



THE FOLLOWING  22 STATION OBSERVATIONS WERE WITHIN THE GRID

  1   +101     1       744.180 4279.860     .36100E-01
  2   +102     2       742.520 4286.050     .65700E-01
  3   +103     3       747.590 4282.470     .15000E-01
  4   +106     6       738.660 4277.570     .25000E-02
  5   +107     7       740.180 4282.610     .32600E-01
  6   +108     8       748.410 4291.100     .10600E-01
  7   +109     9       755.800 4279.890     .67100E-02
  8   +110    10       747.210 4272.830     .80000E-02
  9   +111    11       738.810 4272.480     .21200E-01
 10   +112    12       733.940 4280.910     .35400E-01
 11   +113    13       737.740 4289.820     .21300E-01
 12   +114    14       744.320 4297.460     .13700E-01
 13   +115    15       757.110 4297.800     .25000E-02
 14   +116    16       762.780 4290.080     .25000E-02
 15   +117    17       760.560 4272.820     .25000E-02
 16   +118    18       743.070 4263.260     .28600E-02
 17   +119    19       729.760 4270.550     .16400E-01
 18   +120    20       723.080 4285.910     .31400E-01
 19   +121    21       732.410 4302.380     .13900E-01
 20   +123    23       777.320 4286.380     .25000E-02
 21   +124    24       749.280 4236.540     .25000E-02
 22   +125    25       697.450 4282.240     .15300E-01


THE FOLLOWING   0 UTM OBSERVATIONS WERE WITHIN THE GRID
```

```
SURFACE STATION OBSERVATIONS CONVERTED TO AVERAGE

  1   +101     1       744.180 4279.860     .14886E-01
  2   +102     2       742.520 4286.050     .60074E-01
  3   +103     3       747.590 4282.470     .94819E-02
  4   +106     6       738.660 4277.570     .10000E-02
  5   +107     7       740.180 4282.610     .19115E-01
  6   +108     8       748.410 4291.100     .81693E-02
  7   +109     9       755.800 4279.890     .44885E-02
  8   +110    10       747.210 4272.830     .47805E-02
  9   +111    11       738.810 4272.480     .11695E-01
 10   +112    12       733.940 4280.910     .28434E-01
 11   +113    13       737.740 4289.820     .11914E-01
 12   +114    14       744.320 4297.460     .12042E-01
 13   +115    15       757.110 4297.800     .20696E-02
 14   +116    16       762.780 4290.080     .14338E-02
 15   +117    17       760.560 4272.820     .12376E-02
 16   +118    18       743.070 4263.260     .12133E-02
 17   +119    19       729.760 4270.550     .97371E-02
 18   +120    20       723.080 4285.910     .26083E-01
 19   +121    21       732.410 4302.380     .13436E-01
 20   +123    23       777.320 4286.380     .20396E-02
 21   +124    24       749.280 4236.540     .23037E-02
 22   +125    25       697.450 4282.240     .15145E-01
```

```
POLLUTANT  SULFUR DIOXIDE
SOURCE COLUMN  6
MOLECULAR WEIGHT     64.00
BACKGROUND VALUES]  WEST     .1001E-01 EAST     .1001E-01
  SOUTH    .1001E-01 NORTH    .1001E-01 TOP      .1001E-01



THE FOLLOWING   0 STATION OBSERVATIONS WERE WITHIN THE GRID



THE FOLLOWING   0 UTM OBSERVATIONS WERE WITHIN THE GRID
```

FIGURE H-4. Continued.

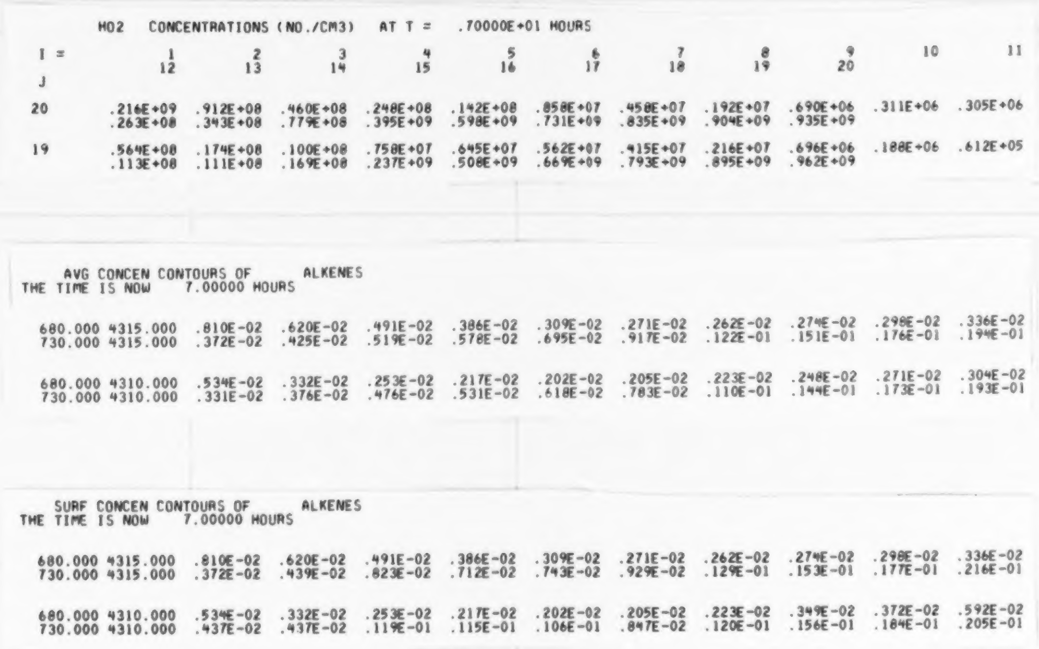
```
     AVG CONCEN CONTOURS OF         SULFUR DIOXIDE
THE TIME IS NOW    6.00000 HOURS

  680.000 4315.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01
  730.000 4315.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01

  680.000 4310.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01
  730.000 4310.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01

  680.000 4305.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01
  730.000 4305.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01

  680.000 4300.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01
  730.000 4300.000  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01  .100E-01
```

```
     SURF CONCEN CONTOURS OF        SULFUR DIOXIDE
THE TIME IS NOW    6.00000 HOURS

  680.000 4315.000  .530E-02  .537E-02  .544E-02  .564E-02  .599E-02  .621E-02  .632E-02  .643E-02  .641E-02  .640E-02
  730.000 4315.000  .637E-02  .636E-02  .651E-02  .645E-02  .630E-02  .632E-02  .639E-02  .641E-02  .647E-02  .677E-02

  680.000 4310.000  .527E-02  .531E-02  .534E-02  .547E-02  .577E-02  .606E-02  .620E-02  .639E-02  .640E-02  .654E-02
  730.000 4310.000  .644E-02  .651E-02  .654E-02  .644E-02  .629E-02  .626E-02  .637E-02  .654E-02  .663E-02  .667E-02

  680.000 4305.000  .527E-02  .527E-02  .535E-02  .552E-02  .591E-02  .588E-02  .608E-02  .631E-02  .636E-02  .635E-02
  730.000 4305.000  .638E-02  .636E-02  .673E-02  .700E-02  .663E-02  .637E-02  .644E-02  .657E-02  .666E-02  .669E-02
```

```
  680.000 4225.000  .559E-02  .571E-02  .578E-02  .583E-02  .593E-02  .602E-02  .596E-02  .580E-02  .584E-02  .571E-02
  730.000 4225.000   835E-02  .567E-02  .571E-02  .578E-02  .569E-02  .571E-02  .574E-02  .580E-02  .595E-02  .613E-02

  680.000 4220.000  .576E-02  .588E-02  .585E-02  .595E-02  .603E-02  .606E-02  .598E-02  .580E-02  .578E-02  .571E-02
  730.000 4220.000  .576E-02  .571E-02  .570E-02  .567E-02  .570E-02  .579E-02  .569E-02  .574E-02  .586E-02  .605E-02
  .1000E-01    .2160E+05    .9000E+03
  .1000E+00    .2160E+05    .9000E+03
  .1000E+01    .2160E+05    .9000E+03
  .2854E+01    .2161E+05    .9000E+03
  .5897E+01    .2162E+05    .9000E+03
  .1021E+02    .2165E+05    .9000E+03
  .1544E+02    .2170E+05    .9000E+03
  .2389E+02    .2177E+05    .9000E+03
  .4614E+02    .2189E+05    .9000E+03
  .7910E+02    .2212E+05    .9000E+03
  .1110E+03    .2252E+05    .9000E+03
  .1651E+03    .2308E+05    .9000E+03
CONCENTRATIONS WRITTEN AT T =     .2340E+05
```

```
                                                       .70000E+01 HOURS
 T =  .25200E+05  H =  .28887E+03 NQ =   3  NFE =   92  NSTEP =   65

PHOTO-DISSOCIATION RATES

   .61E-02   .11E-02   .85E-06   .94E-05   .95E-03   .94E-05   .22E-02   .35E-03   .17E-05

 STEADY STATE SPECIES IN ZONE 1,1

 O3P    .6565249766152E+04
 NO3    .2329687324554E+08
 HO     .1112297427291E+07
 RO     .7299807691314E+04
 N2O5   .1846161203701E+08
 RCO3   .8987410711895E+08
 RO2    .1507859057702E+10
 HO2    .1000509582389E+10

DYNAMIC SPECIES IN ZONE 1,1

HC1    .4847476118082E+12
HC2    .5132071550165E+12
HC4    .1439886595139E+12
HNO2   .2941021242277E+08
HNO3   .6524063634461E+09
H2O2   .4322560015531E+10
NO     .7222935112989E+10
NO2    .4277252199816E+11
O3     .1262300649741E+13
CO     .2556390049445E+13
SO2    .2453416225930E+12
SO4=   .2514786599366E+11
```

FIGURE H-4. Continued.

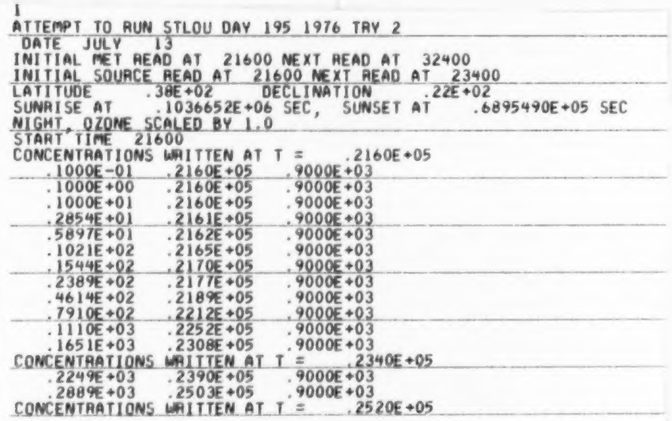


```
        HO2   CONCENTRATIONS (NO./CM3)   AT T =    .70000E+01 HOURS

 I =             1          2          3          4          5          6          7          8          9         10         11
                12         13         14         15         16         17         18         19         20
 J

20           .216E+09   .912E+08   .460E+08   .248E+08   .142E+08   .858E+07   .458E+07   .192E+07   .690E+06   .311E+06   .305E+06
             .263E+08   .343E+08   .779E+08   .395E+09   .598E+09   .731E+09   .835E+09   .904E+09   .935E+09

19           .564E+08   .174E+08   .100E+08   .758E+07   .645E+07   .562E+07   .415E+07   .216E+07   .696E+06   .188E+06   .612E+05
             .113E+08   .111E+08   .169E+08   .237E+09   .508E+09   .669E+09   .793E+09   .895E+09   .962E+09
```

```
     AVG CONCEN CONTOURS OF      ALKENES
 THE TIME IS NOW    7.00000 HOURS

   680.000 4315.000  .810E-02  .620E-02  .491E-02  .386E-02  .309E-02  .271E-02  .262E-02  .274E-02  .298E-02  .336E-02
   730.000 4315.000  .372E-02  .425E-02  .519E-02  .578E-02  .695E-02  .917E-02  .122E-01  .151E-01  .176E-01  .194E-01

   680.000 4310.000  .534E-02  .332E-02  .253E-02  .217E-02  .202E-02  .205E-02  .223E-02  .248E-02  .271E-02  .304E-02
   730.000 4310.000  .331E-02  .376E-02  .476E-02  .531E-02  .618E-02  .783E-02  .110E-01  .144E-01  .173E-01  .193E-01
```

```
     SURF CONCEN CONTOURS OF      ALKENES
 THE TIME IS NOW    7.00000 HOURS

   680.000 4315.000  .810E-02  .620E-02  .491E-02  .386E-02  .309E-02  .271E-02  .262E-02  .274E-02  .298E-02  .336E-02
   730.000 4315.000  .372E-02  .439E-02  .823E-02  .712E-02  .743E-02  .929E-02  .129E-01  .153E-01  .177E-01  .216E-01

   680.000 4310.000  .534E-02  .332E-02  .253E-02  .217E-02  .202E-02  .205E-02  .223E-02  .349E-02  .372E-02  .592E-02
   730.000 4310.000  .437E-02  .437E-02  .119E-01  .115E-01  .106E-01  .847E-02  .120E-01  .156E-01  .184E-01  .205E-01
```

FIGURE H-4. Continued.



```
1
ATTEMPT TO RUN STLOU DAY 195 1976 TRY 2
 DATE  JULY   13
INITIAL MET READ AT  21600 NEXT READ AT  32400
INITIAL SOURCE READ AT  21600 NEXT READ AT  23400
LATITUDE      .38E+02     DECLINATION      .22E+02
SUNRISE AT    .1036652E+06 SEC,  SUNSET AT    .6895490E+05 SEC
NIGHT, OZONE SCALED BY 1.0
START TIME  21600
CONCENTRATIONS WRITTEN AT T =     .2160E+05
    .1000E-01    .2160E+05    .9000E+03
    .1000E+00    .2160E+05    .9000E+03
    .1000E+01    .2160E+05    .9000E+03
    .2854E+01    .2161E+05    .9000E+03
    .5897E+01    .2162E+05    .9000E+03
    .1021E+02    .2165E+05    .9000E+03
    .1544E+02    .2170E+05    .9000E+03
    .2389E+02    .2177E+05    .9000E+03
    .4614E+02    .2189E+05    .9000E+03
    .7910E+02    .2212E+05    .9000E+03
    .1110E+03    .2252E+05    .9000E+03
    .1651E+03    .2308E+05    .9000E+03
CONCENTRATIONS WRITTEN AT T =     .2340E+05
    .2249E+03    .2390E+05    .9000E+03
    .2889E+03    .2503E+05    .9000E+03
CONCENTRATIONS WRITTEN AT T =     .2520E+05
```

FIGURE H-5. Sample LIRAQ-2S QSTEP output.

APPENDIX I

VERF

The post-processor, VERF, compares observed species concentrations read from a QICON file with concentrations computed by LIRAQ-1S or LIRAQ-2S as recorded on a QSREC file. The only other input file is the control card deck. Attached to the control card deck are a few lines of code input that set run parameters for VERF.

The files associated with VERF are listed in Table I-1. The input files to VERF are just the QICON and QSREC files involved in a given LIRAQ run. There are, however, some restrictions on QSREC content if a QSREC is to be used with VERF that are more restrictive than the conditions involved in a normal LIRAQ run.

1. The LIRAQ run must produce station edits every 30 minutes.
2. The LIRAQ run must produce QSREC output at no more than 25 stations and UTM locations.
3. The LIRAQ run must not exceed 24 hours.

TABLE I-1. Files associated with VERF.

File name	Content	Source	Where described
QSREC	Computed concentrations at selected stations	LIRAQ-1S or LIRAQ-2S	Appendix G
QICON	Measured concentrations	QPROC	Appendix D and MASCON User's Guide
VERFLGO	Control card deck	User	Appendix J
OUTPUT	Diagnostic warning message	VERF	Below
GRAPHICS	Graphical display of verification statistics	VERF	Below

4. The LIRAQ run must not output more pollutants than HC1, HC2, HC4, NO, NO_2, O_3, CO and SO_2 to QSREC.

VERF run parameters are input through the control card deck, discussed in Appendix J.

The output file OUTPUT contains error messages and other diagnostic messages from the FTN compiler and the LBL systems libraries. The output file GRAPHICS contains plots of measured and computed concentrations vs. time for every station and pollutant specified in the control card deck and covered by both QSREC and QICON. On these plots the mean and variance for the observed and computed concentrations, the correlation coefficient and the RMS error are given. After all stations reporting a given pollutant have been plotted against time, scatter diagrams are given for all the individual points, and for the means and maxima at the individual observing stations. Following this is a histogram of the frequency of occurrence of error vs. the error. Samples of VERF graphical output are given in Figs. I-1 to I-8.

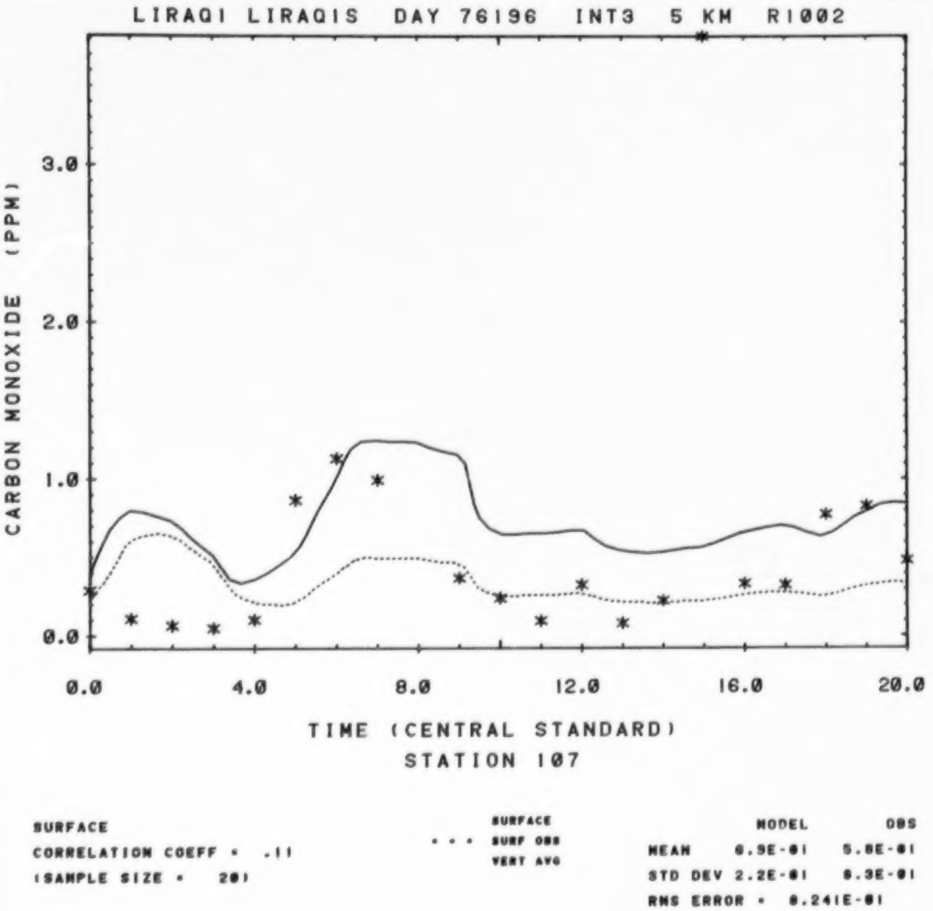
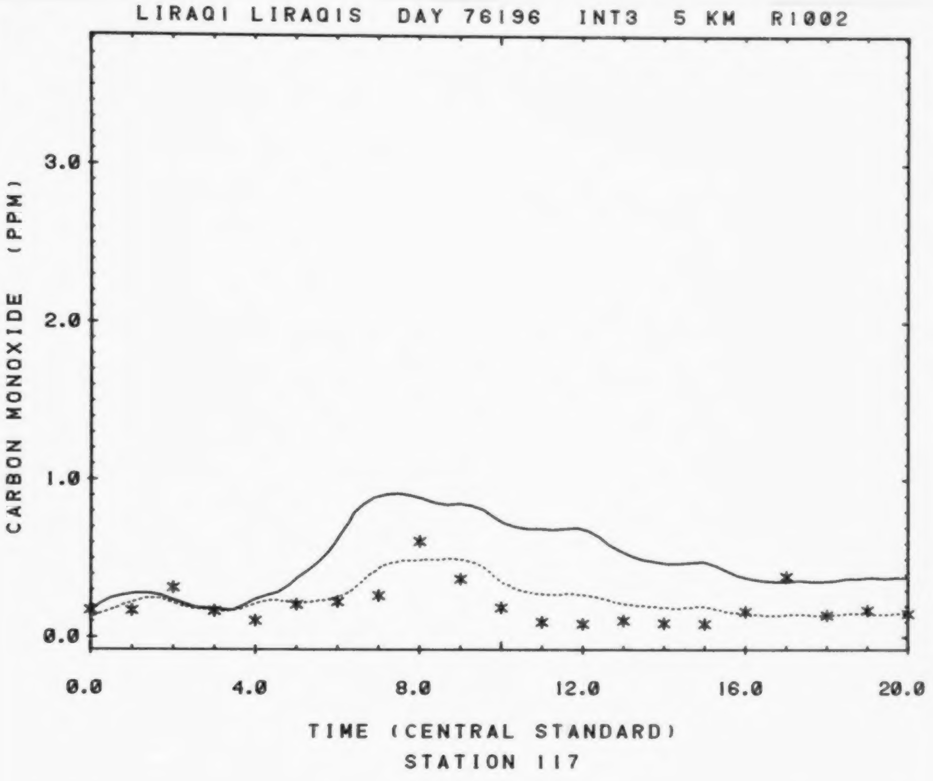


FIGURE I-1. Sample of VERF output — comparison of model and observation at station 107. The solid line gives calculated concentrations 1 m above the surface, the dotted line gives concentrations calculated averaged over the mean layer, and the asterisks give the concentrations measured at monitoring stations. The measured point at 1500 is at the upper boundary of the plot. There is at least some possibility that it reflects a keypunching error in the RAPS data base, if so the agreement between model and observation would be greatly improved.



```
SURFACE                                  SURFACE                   MODEL       OBS
CORRELATION COEFF =  .30           * * * SURF OBS     MEAN     4.9E-01   2.0E-01
(SAMPLE SIZE =   21)                     VERT AVG     STD DEV 2.3E-01   1.3E-01
                                                      RMS ERROR =  3.520E-01
```

FIGURE I-2. Sample of VERF output — comparison of model and observation at station 117.

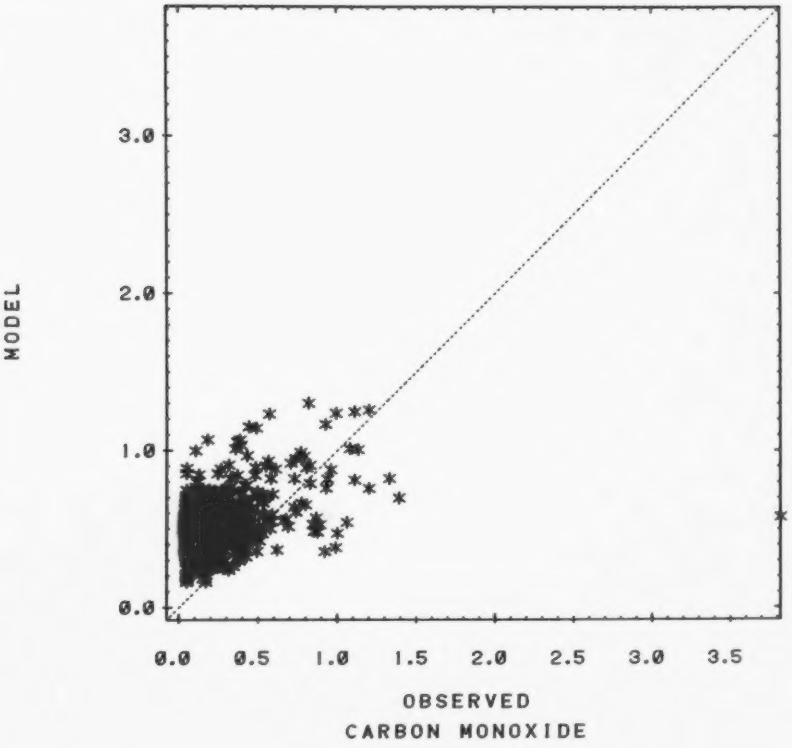


FIGURE I-3. Scatter diagram of all model and observed CO points for day 76 196. All but one of the data points is within 1 ppm of the model prediction. The one deviant point may reflect an error in the RAPS data base.

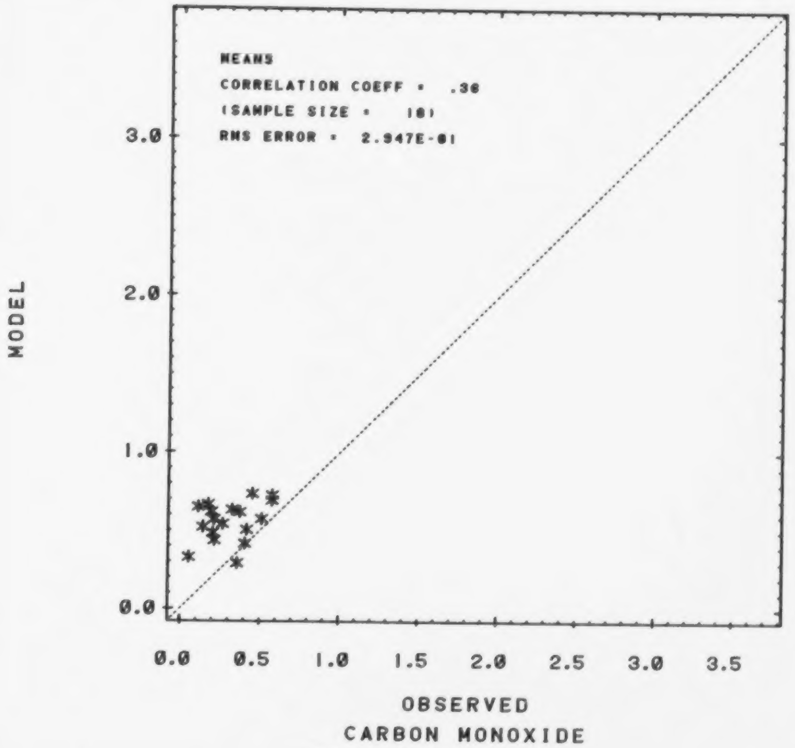


FIGURE I-4. Scatter diagram of observed and calculated mean CO concentrations at stations.

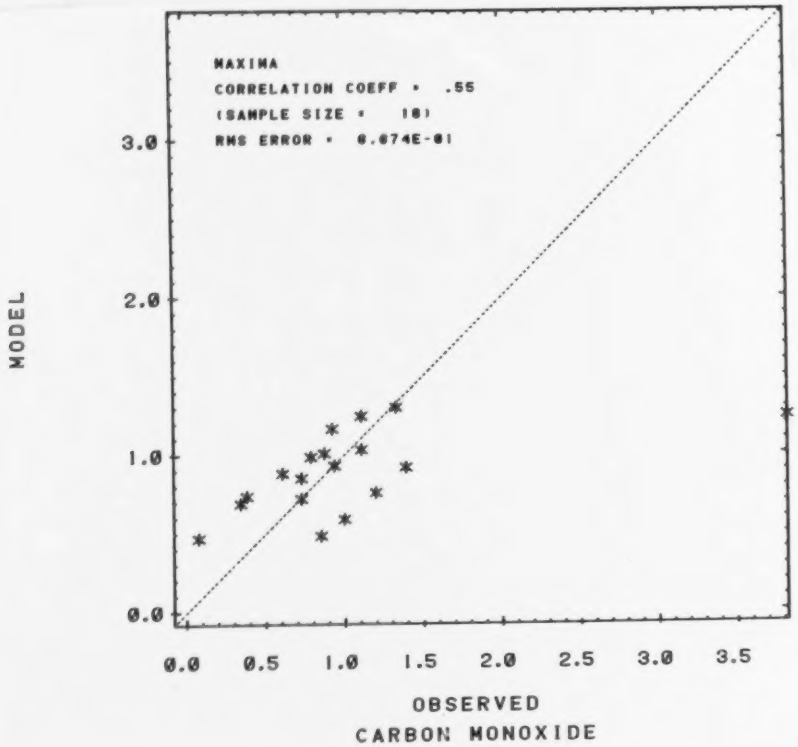


FIGURE I-5. Scatter diagram of observed and calculated maximum CO concentrations at stations.

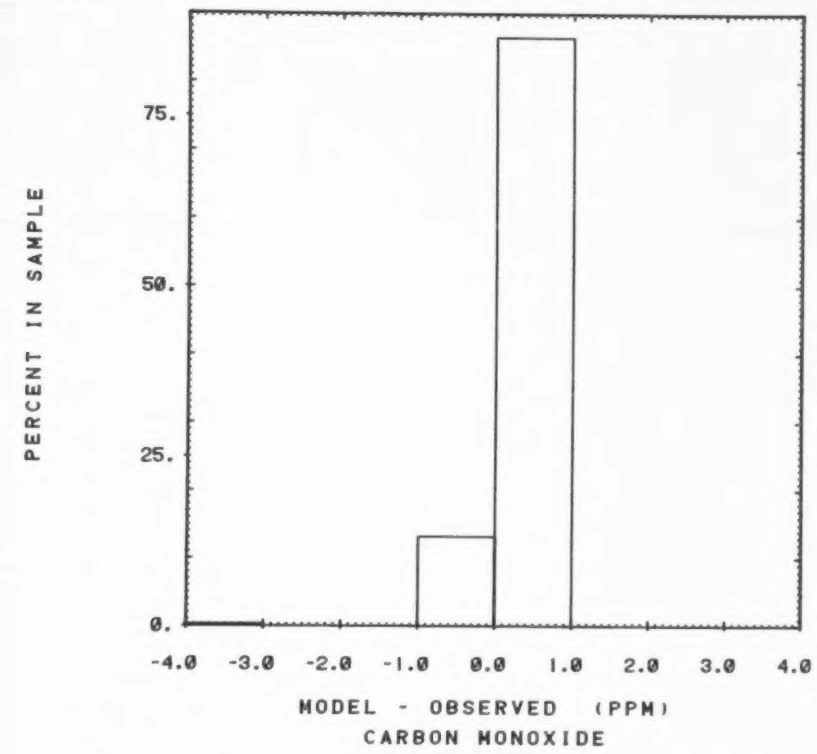


FIGURE I-6. Histogram of model error for CO.

```
           CARBON MONOXIDE

SURFACE
CORRELATION COEFF =   .08
(SAMPLE SIZE =  333)
             MODEL        OBS
MEAN     4.7E-01    3.1E-01
STD DEV 2.8E-01    3.3E-01
RMS ERROR =  4.480E-01
```

FIGURE I-7. Summary of statistics for CO based on all observations.

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
BEGIN LAST LINE OF TEXT HERE
BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"
PAGE NUMBER
EPA-287 (Cin.)
(4-76)

```
AVG CORRELATION COEFFICIENT FOR  CARBON MONOXIDE    =  .46
(SAMPLE SIZE =  333)
AVG CORRELATION COEFFICIENT FOR  ALKANES            = 0.
(SAMPLE SIZE =    0)
AVG CORRELATION COEFFICIENT FOR  NITROGEN DIOXIDE   = 0.
(SAMPLE SIZE =    0)
AVG CORRELATION COEFFICIENT FOR  NITRIC OXIDE       = 0.
(SAMPLE SIZE =    0)
AVG CORRELATION COEFFICIENT FOR  OZONE              = 0.
(SAMPLE SIZE =    0)
AVG CORRELATION COEFFICIENT FOR  SULFUR DIOXIDE     = 0.
(SAMPLE SIZE =    0)
AVG CORRELATION COEFFICIENT FOR ALL POLLUTANTS =   .46
(SAMPLE SIZE =  333)
```

FIGURE I-8. Average of correlation coefficients at stations.

APPENDIX J

CONTROL CARD DECKS

This appendix contains sample control card decks used in executing and compiling the various codes associated with the LIRAQ models along with a brief discussion of necessary modification of these control card decks on the LBL system.

The precise content of these decks is a function of the computer system and compilers in use at any given time. Future changes in the LBL computer system may require changes in the content of some of these files, indeed several files have needed to be changed since January 1, 1979.

Figure J-1 lists a sample control card deck for the source processor. Five types of cards must be altered before the source processor can be used. These cards are:

1. Job Card — This card should have a short job name, a priority, computing limit, your valid LBL account, and your name.
2. Routing Information — This card will presently send output to W. H. Duewer at LLL. It should have your address.
3. Title Card — The title should be altered to whatever you wish to appear as a run title.
4. Data Retrieval — The first STAGE card reads a binary area source file. The file to be secured is determined by its position on the tape. The second STAGE card reads a binary point source file. Again the file is identified by its position on the tape. See LBL documentation of STAGE for a discussion of the arguments.
5. Data Storage — The STOTAPE commands should be altered so that the QSORxx files are archived on your tape with the address structure you desire.

Figure J-2 gives a sample of QPRCLGO, the control card deck that executes the Q-Processor. The following five changes should be made.

1. Job Card — The job card should be given your name and account number.
2. Routing Information — The routing instructions should contain your address.
3. Title Card — The title should be altered to whatever you wish to appear as a run title.

```
(1) SPRC,7,1600.679656,GRANT,K
    *HOLDOUT
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .# SOURCE PROCESSOR EXECUTION 781121
    .**** THE PRECEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE RUN TITLE FOR LABELING OF OUTPUT.
    ..
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    ..
    .  AVAILABILITY...
    .        THIS CONTROL CARD DECK CAN BE OBTAINED BY EXECUTING THE
    .        FOLLOWING CONTROL CARD
    .           LIBCOPY, SORPROC, SPRCLGO, SPRCLGO.
    ..
    .  PURPOSE...
    .        THIS CONTROL CARD DECK PERFORMS THE SOURCE PROCESSOR EXECUTION
    .        PROCESS.  IN ADDITION TO AND BEFORE THE EXECUTION OF THE
    .        SOURCE PROCESSOR, THIS PROCESS INCLUDES EXECUTION OF 'READAR'
    .        AND 'READPT' TO CONVERT AREA AND POINT SOURCE BINARY FILES
    .        INTO CARD IMAGE FILES.  THE SOURCE PROCESSOR INPUTS THESE CARD
    .        IMAGE FILES AND OUTPUTS A 'QSOR' FILE FAMILY.
    ..
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    ..
    DISKHOG, 20000.
    .....GET THE AREA SOURCE BINARY FILE FROM TAPE
    .**** THE FOLLOWING CARD IS RUN DEPENDENT
(4) STAGE, AREABN, 27349, 2FS, 1F, MT.
    ..
    ..... EXECUTE READAR TO PRODUCE A CARD IMAGE AREA SOURCE FILE
    FETCHPS, SORPROC, RDARBN, RDARBN.
    LINK, F=RDARBN, L=0, RF, X.
    RETURN, AREABN.
    EXIT.
    FETCHPS, SORPROC, RDARSYM, RDARSYM.
    GRUMP, P=RDARSYM.
    RETURN, RDARSYM.
    DISPOSE, AREA=MF, T=[AREA SOURCES].
    BGNSKIP.
    CXIT.
    BGNSKIP.
    FIN.
    ..
    ..... GET THE POINT SOURCE BINARY FILE FROM TAPE.
    .**** THE FOLLOWING CARD IS RUN DEPENDENT
(4) STAGE, PBIN, 28229, 1FS, 1F, MT.
    ..
    ..... EXECUTE READPT TO PRODUCE A CARD IMAGE POINT SOURCE FILE
    FETCHPS, SORPROC, RDPTBN, RDPTBN.
    LINK, F=RDPTBN, L=0, RF, X.
    RETURN, PBIN.
    EXIT.
    FETCHPS, SORPROC, RDPTSYM, RDPTSYM.
    GRUMP, P=RDPTSYM.
    RETURN, RDPTSYM.
    DISPOSE, POINT=MF, T=[POINT SOURCES].
    BGNSKIP.
    CXIT.
    BGNSKIP.
    FIN.
```

FIGURE J-1. Sample of SPRCCGO, the control cards that run the source processor.

```
..
..... EXECUTE THE SOURCE PROCESSOR
REWIND, AREA.
REWIND, POINT.
LIBCOPY, SORPROC, INPUTS, SPRCINP.
LIBCOPY, SORPROC, GRIDES, GRIDES.
LIBCOPY, SORPROC, SPRCBN, SPRCBN.
LINK, F=SPRCBN, L=0, RF, X.
RETURN, INPUTS, GRIDES.
EXIT.
FETCHPS, SORPROC, SPRCSYM, SPRCSYM.
GRUMP, P=SPRCSYM.
RETURN, SPRCSYM.
CXIT.
FIN.
```

(5)

```
..
..... ARCHIVE THE 'QSOR' FILES ON TAPE
DISPOSE, AREA=MF, CC=SS,  T=[AREA SOURCES].
DISPOSE, POINT=MF, CC=SS,  T=[POINT SOURCES].
DETECT, QSOR00.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR00, 16449.].
DETECT, QSOR01.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR01, 16449.].
DETECT, QSOR02.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR02, 16449.].
DETECT, QSOR03.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR03, 16449.].
DETECT, QSOR04.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR04, 16449.].
DETECT, QSOR05.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR05, 16449.].
DETECT, QSOR06.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR06, 16449.].
DETECT, QSOR07.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR07, 16449.].
DETECT, QSOR08.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR08, 16449.].
DETECT, QSOR09.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR09, 16449.].
DETECT, QSOR10.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR10, 16449.].
DETECT, QSOR11.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR11, 16449.].
DETECT, QSOR12.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR12, 16449.].
DETECT, QSOR13.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR13, 16449.].
DETECT, QSOR14.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR14, 16449.].
DETECT, QSOR15.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR15, 16449.].
DETECT, QSOR16.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR16, 16449.].
DETECT, QSOR17.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR17, 16449.].
DETECT, QSOR18.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR18, 16449.].
DETECT, QSOR19.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR19, 16449.].
DETECT, QSOR20.
TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR20, 16449.].
DETECT, QSOR21.
```

FIGURE J-1. Continued.

```
    [ TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR21, 16449.].
    | DETECT, QSOR22.
    | TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR22, 16449.].
(5) | DETECT, QSOR23.
    | TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR23, 16449.].
    | DETECT, QSOR24.
    [ TEXT, TEMP, [STOTAPE, DAY76195/GS5KM/QSOR24, 16449.].
      CXIT.
      FIN.
      COPY, TEMP/RX, OFXB, STOCTRL/RR.
      CALL, STOCTRL.
      RETURN, STOCTRL.
      ..
      DISPOSE, QSOR00=MF, T=[QSOR00].
      DISPOSE, QSOR01=MF, T=[QSOR01].
      DISPOSE, QSOR02=MF, T=[QSOR02].
      DISPOSE, QSOR03=MF, T=[QSOR03].
      DISPOSE, QSOR04=MF, T=[QSOR04].
      DISPOSE, QSOR05=MF, T=[QSOR05].
      DISPOSE, QSOR06=MF, T=[QSOR06].
      DISPOSE, QSOR07=MF, T=[QSOR07].
      DISPOSE, QSOR08=MF, T=[QSOR08].
      DISPOSE, QSOR09=MF, T=[QSOR09].
      DISPOSE, QSOR10=MF, T=[QSOR10].
      DISPOSE, QSOR11=MF, T=[QSOR11].
      DISPOSE, QSOR12=MF, T=[QSOR12].
      DISPOSE, QSOR13=MF, T=[QSOR13].
      DISPOSE, QSOR14=MF, T=[QSOR14].
      DISPOSE, QSOR15=MF, T=[QSOR15].
      DISPOSE, QSOR16=MF, T=[QSOR16].
      DISPOSE, QSOR17=MF, T=[QSOR17].
      DISPOSE, QSOR18=MF, T=[QSOR18].
      DISPOSE, QSOR19=MF, T=[QSOR19].
      DISPOSE, QSOR20=MF, T=[QSOR20].
      DISPOSE, QSOR21=MF, T=[QSOR21].
      DISPOSE, QSOR22=MF, T=[QSOR22].
      DISPOSE, QSOR23=MF, T=[QSOR23].
      DISPOSE, QSOR24=MF, T=[QSOR24].
      CXIT.
      EXIT.
      FIN.
      ENDSKIP.
      ..
      ..... CREATE A MICROFICHE ARCHIVE OF THIS RUN
      TIM.
      DDB.
      REWIND, DAYFILE.
      FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
      FISHTLT, DAYFILE.
      RETURN, FISHTLT.
      ..
      TEXT, ARCHIVE, [$B=DAYFILE].
      COPY, DAYFILE/RX, ARCHIVE.
      ..
      TEXT, ARCHIVE, [$CL].
      TEXT, ARCHIVE, [$B=INPUT].
      REWIND, INPUT.
      COPYSBF, INPUT, ARCHIVE.
      RETURN, INPUT.
      ..
      TEXT, ARCHIVE, [$CL].
      TEXT, ARCHIVE, [$B=OUTPUT].

      COPY, OUTPUT/RB, ARCHIVE.
      ..
      CXIT.
      EXIT.
      FIN.
      DISPOSE, ARCHIVE=MF,
      + T1=[→R0→R1→R2→R3→R4→R5],
      + T2=[→R6→R7→R8→R9].
      END.
```

FIGURE J-1. Continued.

```
(1) QPRC,16,100.679656,GRANT,K
    *HOLDOUT
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .# Q-PROCESSOR RUN, QPMET GENERATION
    .**** THE ABOVE TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE RUN TITLE FOR LABELING OF OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .         THIS CONTROL DECK EXECUTES THE Q-PROCESSOR (QPROC), A DATA
    .         PREPROCESSOR FOR THE MASCON AND LIRAQ MODELS.  QPROC IS
    .         WRITTEN IN THE PASCAL LANGUAGE.  IT READS CONCENTRATION
    .         AND METEOROLOGICAL DATA FROM THE RAMS DATA FILE (RAMSDAT)
    .         AND READS USER CONTROL INFORMATION FROM THE FILE QPINPUT.
    .         FROM THIS DATA, QPROC GENERATES AN INITIAL CONCENTRATION FILE
    .         (QICON) AND A METEOROLOGICAL DATA FILE (QPMET).  THE QPMET
    .         FILE IS INTENDED TO BE USED AS INPUT TO THE M-PROCESSOR
    .         (MPROC), ANOTHER PREPROCESSOR FOR THE MASCON MODEL.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    ..... GET THE MIXING HEIGHT FILE, THE RAMS DATA FILE, AND THE
    ..... Q-PROCESSOR INPUT FILE FROM TAPE
    .**** THE FOLLOWING THREE FETCHGS CARDS ARE RUN DEPENDENT - CHANGE THE
    .**** DIRECTORY PATH NAMES AND/OR THE TAPE NAME(S).
  [ FETCHGS, DAY76195/MIXHGT,  16449.
  | FETCHGS, DAY76195/RAMSDAT, 16449.
  | FETCHGS, DAY76195/QPINPUT, 16449.
(4) .
  | ..... GET THE OTHER FILES NECESSARY TO RUN THE Q-PROCESSOR
  | FETCHPS, PASCAL, PASLIB, PASLIB.
  | FETCHPS, MASCON, LGO, QPRCBN.
  L FETCHPS, MASCON, QPMET, QPMCOM.
    .
    ..... RUN THE Q-PROCESSOR, GENERATING A QICON FILE AND A QPMET FILE
    SFL, 100000.
    LINK, FL=0, L=0, P=PASLIB, RF, X, PP=[QPINPUT].
    RETURN, MIXHGT, RAMSDAT.
    .
    .
    ..... SAVE THE QICON FILE AND THE QPMET FILE ON TAPE
    .**** THE FOLLOWING THREE CARDS ARE RUN DEPENDENT - CHANGE
    .**** THE DIRECTORY PATH NAMES AND/OR THE TAPE NAME(S).
  [ STOTAPE, DAY76195/QICON, 16449.
(5) STOTAPE, DAY76195/QPMET, 16449.
  L ENTERGS, DAY76195/QPMET, 16449.
    .
    .
    ..... CREATE AN ARCHIVE FILE OF THIS RUN FOR OUTPUT AS MICROFICHE
    CXIT.
    EXIT.
    FIN.
    TIM.
    DDB.
    REWIND, DAYFILE.
    FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
    FISHTLT, DAYFILE.
    RETURN, FISHTLT.
    .
```

FIGURE J-2. Sample of QPRCCGO, the control cards that execute the Q-processor.

```
TEXT, ARCHIVE, [$B=DAYFILE].
COPY, DAYFILE/RX, ARCHIVE.
.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=INPUT].
REWIND, INPUT.
COPYSBF, INPUT, ARCHIVE.
RETURN, INPUT.
.
TEXT, ARCHIVE, [$B=OUTPUT].
COPY, OUTPUT/RB, ARCHIVE.
.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QPINPUT].
REWIND, QPINPUT.
COPYSBF, QPINPUT, ARCHIVE.
RETURN, QPINPUT.
.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QICON].
REWIND, QICON.
COPYSBF, QICON, ARCHIVE.
RETURN, QICON.
.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QPMET].
REWIND, QPMET.
COPYSBF, QPMET, ARCHIVE.
RETURN, QPMET.
.
CXIT.
EXIT.
FIN.
DISPOSE, ARCHIVE=MF,
+ T1=[→R0→R1→R2→R3→R4→R5],
+ T2=[→R6→R7→R8→R9].
END.
```

FIGURE J-2. Continued.

4. Data Retrieval — The FETCHGS cards that assemble MIXHGT, RAMSDAT and QPINPUT should be replaced by cards that read data from your archive. In all likelihood MIXHGT and RAMSDAT should be read from a tape, and those FETCHGS cards replaced with STAGE or GETTAPE cards.

5. Data Storage — The STOTAPE and ENTERGS cards should be altered to store QICON and QPMET in your archive.

Figure J-3 gives a sample of MPRCLGO, the control card deck that executes the M-Processor. The following cards must be changed:

1. Job Card — The job card must be given your name and account number.
2. Routing Information — The routing card must be given your address.
3. Title Card — The title should be altered to whatever you want.
4. Data Retrieval — The FETCHGS card that retrieves QPMET should be altered to acquire the QPMET you wish to use.
5. Data Storage — The STOTAPE and ENTERGS cards that dispose of QMET should be altered to reflect the structure of your archive
6. The three cards at the end of the deck should be altered to contain.
    a. The start time (hour, Julian date, year (Format — 6X,I2,1X,I3,1X,I4)).
    b. The stop time (hour, date, year (Format — 6X,I2,1X,I3,1X,I4)).
    c. The interval between QMET (output) intervals (hours) (Format — 9X,I2).

Figure J-4 lists a simple UADCGO. This deck compiles, loads, and executes UADATA. The following cards should be modified:

1. Job Card — The job card should be given your name and LBL account number.
2. Routing Information — The routing instructions should be given your address.
3. Title Card — The title should be altered to describe your run.
4. Data Retrieval — The GETTAPE card that retrieves the RAMS file should be altered to retrieve the data you want to display.
5. The last card should be altered to contain the hours of the day that you wish to display (25I2 Format) -1 is a sentinal for end of data. The card on the sample will display all data in a given RAMS file even if some hours are missing from the input file.

```
(1)  MPRC,16,100.679656,GRANT,K
     *HOLDOUT
(2)  (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3)  .≠ M-PROCESSOR RUN, QMET GENERATION
     .**** THE ABOVE TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
     .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
     .**** CARD CONTAINS THE RUN TITLE FOR LABELING OF OUTPUT.
     .
     .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
     .
     .         THIS CONTROL DECK EXECUTES THE M-PROCESSOR (MPROC), A DATA
     .         PREPROCESSOR FOR THE MASCON MODEL.  MPROC IS WRITTEN IN FTN4
     .         FORTRAN.  IT READS CONTROL INFORMATION FROM THE FILE INPUT
     .         AND METEOROLOGICAL DATA FROM THE FILE QPMET.  FROM THIS DATA,
     .         MPROC GENERATES A METEOROLOGICAL DATA FILE, QMET, WHICH
     .         IS INTENDED TO BE USED AS INPUT TO THE MASCON MODEL.
     .
     .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
     .
     ..... GET THE QPMET FILE FROM TAPE
     .**** THE FOLLOWING FETCHGS CARD IS RUN DEPENDENT - CHANGE THE
     .**** DIRECTORY PATH NAMES AND/OR THE TAPE NAME.
(4)  FETCHGS, DAY76195/QPMET, 16449.
     .
     .
     ..... RUN THE M-PROCESSOR, GENERATING A QMET FILE
     FETCHPS, MASCON, LGO, MPRCBN.
     LINK, L=0, RF, X.
     RETURN, QPMET.
     .
     .
     ..... SAVE THE QMET FILE ON TAPE
     .**** THE FOLLOWING TWO CARDS ARE RUN DEPENDENT - CHANGE THE
     .**** DIRECTORY PATH NAMES AND/OR THE TAPE NAME.
(5)  STOTAPE, DAY76195/INTERVAL3/QMET, 16449.
     ENTERGS, DAY76195/INTERVAL3/QMET, 16449.
     .
     .
     ..... CREATE AN ARCHIVE FILE OF THIS RUN FOR OUTPUT ON MICROFICHE
     CXIT.
     EXIT.
     FIN.
     TIM.
     DDB.
     REWIND, DAYFILE.
     FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
     FISHTLT, DAYFILE.
     RETURN, FISHTLT.
     .
     TEXT, ARCHIVE, [$B=DAYFILE].
     COPY, DAYFILE/RX, ARCHIVE.
     .
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=INPUT].
     REWIND, INPUT.
     COPYSBF, INPUT, ARCHIVE.
     RETURN, INPUT.
     .
     TEXT, ARCHIVE, [$B=OUTPUT].
     COPY, OUTPUT/RB, ARCHIVE.
     .
```

FIGURE J-3. Sample of MPRCLGO, the control cards that execute the M-processor.

```
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=QMET].
     REWIND, QMET.
     COPYSBF, QMET, ARCHIVE.
     RETURN, QMET.
     .
     CXIT.
     EXIT.
     FIN.
     DISPOSE, ARCHIVE=MF,
     + T1=[→R0→R1→R2→R3→R4→R5],
     + T2=[→R6→R7→R8→R9].
     END.
     ..
     .**** THE CARDS IN THE FOLLOWING RECORD ARE RUN PARAMETER CARDS
     .**** INPUT BY THE M-PROCESSOR, AND MUST BE CHANGED BY THE USER
     .**** AS NECESSARY.
    [START 00 195 1976
(6) [STOP  23 195 1976
    [INTERVAL 03
```

FIGURE J-3. Continued.

```
    1
(1) UAD,05,1200.679656,GRANT,K
    *HOLDOUT
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .* MET DATA PLOTS
    DISKHOG,20000.
    .COPY CONTROL CARD DECK TO OUTPUT LISTING
    REWIND,INPUT.
    COPY,INPUT,1R,CNTR/RR.
    COPYSBF,CNTR,OUTPUT.
    DELETE,CNTR.
    .  SORT OUT THE INPUT
    .INSERT UADDK IN INPUT AFTER CONTROL CARDS AND LEAVE INPUT POSITIONED
    .AT START OF UADDK. THIS IS A SPECIAL TREATMENT.
    FETCHPS,EPA,UADDK,UADDK.
    COPY,INPUT,1R,INPT.
    REWIND,INPUT.
    SKIPR,INPUT,1.
    COPY,UADDK/RX,3R,INPUT.
    COPY,INPT/RX,INPUT.
    REWIND,INPUT.
    SKIPR,INPUT,1.
    ..
    ..    GET THE 'UAD' PROGRAM
    FETCHPS,EPA,OLDPL,METGRAF.
    UPDATE,F,LC=5000,O=UPDOUT,D.
    FTN4,I=COMPILE,R=3.
    CXIT.
    END.
    FIN.
    ..       MAKE SOME MODS TO SOME 'IDDS' ROUTINES
(4) GETTAPE,IDDSTST/OLDPL,V=9,16964.
    UPDATE,O=NULL.
    FTN4,I=COMPILE,OPT=2,L=0.
    CXIT.
    FIN.
    .
    . ****************   INPUT FILES
    .GET RAMSDATA FROM ARCHIVE TAPE
    GETTAPE,RAMS=DAY76195/HISTORY,12749.
    ..      GET THE RIVER OUTINE
    COPY,INPUT,1R,RIV/RR.
    ..      GET THE RAPS GRID
    FETCHPS,EPA,RAPS,RAPSGRD.
    .
    . **********************
    .
    ..         GET THE IDDS LIBRARY
    .                          GET THE 'GRAFPAC' C.O.M. DRIVER
    GETTAPE,GPAC=GRAPHIC/SCLGOF,16964,DATE=02DEC78.
    GETTAPE,GR=IDDSTST/ULIB,16964,DATE=02DEC78.
    GETTAPE,SYMTAB=IDDSTST/SYMTAB,16964,DATE=02DEC78.
    RETURN,OLDPL,COMPILE.
    FETCHPS,GRUMP,GRUMP,GRUMP.
    ..
    ..      SET LCM FIELD LENGTH
    RFL,,50000.
    TIM.
    LINK,F=LGO,P=GR,F=GPAC,X.
    EXIT.
    DUMP,0.
```

FIGURE J-4. Sample of UADCLGO, the control card deck that updates, compiles, and executes the meteorological display code.

BEGIN FIRST LINE OF TEXT HERE
TYPING GUIDE SHEET
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD: BEGIN SECTIONS HERE

```
SFL,,0.
..        SYMBOLIC DUMP
GRUMP,P=OUTPUT,P=SYMTAB.
FIN.
SFL,,0.
..      MAKE FCHE COPY OF INPUT FILES
REWIND,RIV,RAMS,RAPS.
COPYSBF,RIV,MF.
DISPOSE,MF=MF,T=[UADATA INPUT FILE - RIV].
RETURN,RIV.
COPYSBF,RAMS,MF.
DISPOSE,MF=MF,T=[UADATA INPUT FILE - RAMS].
RETURN,RAMS.
COPYSBF,RAPS,MF.
DISPOSE,MF=MF,T=[UADATA INPUT FILE - RAPS].
RETURN,RAPS.
..
COPY,UPDOUT/RX,OUTPUT.
.
....  FICHE ARCHIVE (WITH GRAPHICS, COM FILE FILM)
.
.
.
EXIT.
CXIT.
FIN.
TIM.
FILES.
DDB.
REWIND,DAYFILE.
FETCHPS,GRAPHICS,FISHTLT,FISHTLT.
FISHTLT,DAYFILE.
DELETE,FISHTLT.
REWIND,DAYFILE.
TEXT,FILE,[$RU].
TEXT,FILE,[$B=DAYFILE].
COPY,DAYFILE/RX,FILE.
TEXT,FILE,[$CL].
TEXT,FILE,[$B=INPUT].
REWIND,INPUT.
COPYSBF,INPUT,FILE.
TEXT,FILE,[$CL].
TEXT,FILE,[$B=OUTPUT].
COPY,OUTPUT/RB,FILE.
TEXT,FILE,[$NR].
TEXT,FILE,[$CL].
TEXT,FILE,[$ME].
COPY,FILM/RB,FILE.
DISPOSE,FILE=MF,T1=[→R0→R1→R2→R3→R4→R5],
+T2=[→R6→R7→R8→R9].
DISPOSE,FILM=3M,M=ME.
```

1
(5) 00010203040506070809101112131415161718192021222‌3-1
1

FIGURE J-4. Continued.

BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
BEGIN LAST LINE OF TEXT
3/8"

EPA-287 (Cin.)
(4-70)

Figure J-5 lists a sample of MSCNLGO, the deck that executes MASCON. The following cards should be modified before executing this deck.

1. Job Card — The job card should be given your name and LBL account number.

2. Routing Information — The routing instructions should have your address.

3. Title Card — The title should be whatever you want.

4. Data Retrieval — The LIBCOPY, FETCHPS and GETTAPE cards that assemble QMRUN, QGEO, and QMET should be modified to retrieve the files you wish to use.

5. Data Storage — The STOTAPE instructions that store the QTRANx files should be modified to reflect your directory structure.

Figure J-6 gives a sample of LRISLGO, the deck that executes LIRAQ-1S. The following control cards must be altered by the user.

1. Job Card — The job card must have the user's valid LBL account number and name.

2. Routing Information — The routing instructions must be altered to give an appropriate address.

3. Job Title — The title card should be modified to give a useful job title.

4. The card with SCP, A=2600 CU, must be changed to set A to about 300-400 CU less the computing limit set on the job card.

5. Data Retrieval — The cards that assemble QSRUN, QGEO, QICON, QTRANx, and QSORxx files must be modified to access the files you want to use wherever they are archived. Note that the number of QTRANx files and QSORxx files in an archive may vary. If some QSORxx or QTRANx files are nonexistant the GETTAPE cards for those files should be commented out or deleted.

6. Data Storage — The STOTAPE card that stores the QSREC file should be modified to be compatible with the users archive.

Figure J-7 gives a listing of LR25LGO, the control card deck needed to execute LIRAQ-2S. As in the case of LRISLGO, the cards that must be modified are:

1. Job Card — This must have your valid LBL account number and your name.

2. Routing Information — The routing instructions must be given your address.

3. Title Card — The title should be changed to reflect the job you wish to run.

4. The SCP Card — This sets a computing limit that should be about 400 CU less than that on the job card.

```
(1) MSCN,5,3000.679656,GRANT,K
    *HOLDOUT
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .≠ MASCON MODEL EXECUTION
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .     THIS CONTROL DECK EXECUTES THE MASCON MODEL.  CONTROL CARDS TO
    .     OBTAIN THE INPUT FILES, QGEO, QMET, AND QMRUN, AND TO SAVE
    .     THE QTRAN FILE FAMILY CREATED BY MASCON MUST BE CHANGED BY THE
    .     USER AS NECESSARY.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .**** THE FOLLOWING CARD IS RUN DEPENDENT.  IT SETS THE MAXIMUM TIME
    .**** ALLOWED FOR MODEL EXECUTION TO A NUMBER OF COMPUTING UNITS LESS
    .**** THAN THAT SPECIFIED ON THE JOBCARD.  THIS ALLOWS TIME FOR FILE
    .**** HANDLING IN CASE THE TIME LIMIT IS EXCEEDED.
    SCP, A=2600.
    DISKHOG, 10000.
    .
    .
    ..... GET THE INPUT FILES FROM PSS AND MAGNETIC TAPE
    .**** THE FOLLOWING THREE CARDS ARE RUN AND/OR USER DEPENDENT.  THE USER
   [.**** MUST CHANGE THEM TO PROVIDE HIS OR HER OWN INPUT FILES.
   [LIBCOPY, MASCON, QMRUN, QMRUN00.
(4)[FETCHPS, MASCON, QGEO, QGEOSTL.
   [GETTAPE, DAY76195/INTERVAL3/QMET, 16449.
    .
    .
    ..... LOAD AND EXECUTE
    FETCHPS, MASCON, MSCNBN, MSCNBN.
    GETTAPE, SCLGOF=GRAPHIC/SCLGOF, 16964, DATE=02DEC78.
    GETTAPE, ULIB=IDDSTST/ULIB, 16964, DATE=02DEC78.
    GETTAPE, TV80TLB=GRAPHICS/TV80TLB, 16964, DATE=02DEC78.
    LINK, F=MSCNBN, F=SCLGOF, L=0, P=ULIB, P=TV80TLB, RF, X.
    EXIT.
    DUMP, 0.
    FETCHPS, MASCON, MSCNSYM, MSCNSYM.
    GRUMP, P=MSCNSYM.
    REWIND, QMRUN.
    COPYSBF, QMRUN, OUTPUT.
    CXIT.
    FIN.
    SFL, 50000,0.
    SCP, A=0.
    RETURN, DBGMAP, GRUMP, QMET.
    TIM.
    FILES.
    .
    .
    DISPOSE,QHSP=MF,T=[MASCON - QHSP].
    DISPOSE,QFLXCK=MF,T=[MASCON - QFLXCK].
    .
    .
    ..... ARCHIVE QTRAN FILES ON TAPE AND MICROFICHE
    .**** THE FOLLOWING STOTAPE CARDS ARE RUN DEPENDENT. THE USER MUST CHANGE
    .**** THE DIRECTORY PATH NAMES AND/OR THE TAPE NUMBER AS NECESSARY.
```

FIGURE J-5. Sample of MSCNGGO, the file that executes MASCON.

TYPING GUIDE SHEET

```
      DETECT,QTRAN0.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN0,16449.].
      DETECT,QTRAN1.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN1,16449.].
      DETECT,QTRAN2.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN2,16449.].
      DETECT,QTRAN3.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN3,16449.].
      DETECT,QTRAN4.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN4,16449.].
      DETECT,QTRAN5.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN5,16449.].
      DETECT,QTRAN6.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN6,16449.].
(5)   DETECT,QTRAN7.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN7,16449.].
      DETECT,QTRAN8.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN8,16449.].
      DETECT,QTRAN9.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRAN9,16449.].
      DETECT,QTRANA.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRANA,16449.].
      DETECT,QTRANB.
      TEXT,TEMPA,[STOTAPE,DAY76195/INTERVAL3/REGION1/QTRANB,16449.].
      CXIT.
      FIN.
      COPY,TEMPA/RX,OFXB,STOFILE.
      CALL,STOFILE.
      RETURN,STOFILE.
      DISPOSE,QTRAN0=MF,T=[MASCON - QTRAN0].
      DISPOSE,QTRAN1=MF,T=[MASCON - QTRAN1].
      DISPOSE,QTRAN2=MF,T=[MASCON - QTRAN2].
      DISPOSE,QTRAN3=MF,T=[MASCON - QTRAN3].
      DISPOSE,QTRAN4=MF,T=[MASCON - QTRAN4].
      DISPOSE,QTRAN5=MF,T=[MASCON - QTRAN5].
      DISPOSE,QTRAN6=MF,T=[MASCON - QTRAN6].
      DISPOSE,QTRAN7=MF,T=[MASCON - QTRAN7].
      DISPOSE,QTRAN8=MF,T=[MASCON - QTRAN8].
      DISPOSE,QTRAN9=MF,T=[MASCON - QTRAN9].
      DISPOSE,QTRANA=MF,T=[MASCON - QTRANA].
      DISPOSE,QTRANB=MF,T=[MASCON - QTRANB].
      .
      .
      ..... MICROFICHE ARCHIVE OF RUN WITH GRAPHICS
      CXIT.
      EXIT.
      FIN.
      TIM.
      DDB.
      REWIND, DAYFILE.
      FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
      FISHTLT, DAYFILE.
      RETURN, FISHTLT.
      TEXT, ARCHIVE, [$RU].
      TEXT, ARCHIVE, [$B=DAYFILE].
      COPY, DAYFILE/RX, ARCHIVE.
      TEXT, ARCHIVE, [$CL].
      TEXT, ARCHIVE, [$B=INPUT].
      REWIND, INPUT.
      COPYSBF, INPUT, ARCHIVE.
      DELETE, INPUT.
      TEXT, ARCHIVE, [$CL].
```

FIGURE J-5. Continued.

```
TEXT, ARCHIVE, [$B=OUTPUT].
COPY, OUTPUT/RB, ARCHIVE.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QMRUN].
REWIND, QMRUN.
COPYSBF, QMRUN, ARCHIVE.
RETURN, QMRUN.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QDIAG].
COPY, QDIAG/RX, ARCHIVE.
TEXT, ARCHIVE, [$NR].
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QGRAPH].
TEXT, ARCHIVE, [$ME].
COPY, QGRAPH/RB, ARCHIVE.
CXIT.
EXIT.
FIN.
DISPOSE, QGRAPH=35, M=ME.
DISPOSE, ARCHIVE=MF,
+ T1=[→R0→R1→R2→R3→R4→R5],
+ T2=[→R6→R7→R8→R9].
```

FIGURE J-5. Continued.

```
(1) LR1S,5,3000.679656,GRANT,K
    *HOLDOUT
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .# LIRAQ1S MODEL EXECUTION DAY195 5KM FULL
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .     THIS CONTROL DECK EXECUTES THE LIRAQ1S MODEL.  CONTROL CARDS TO
    .     OBTAIN THE INPUT FILES, QGEO AND QSRUN, TO OBTAIN THE QSOR AND
    .     QTRAN INPUT FILE FAMILIES, AND TO SAVE THE OUTPUT FILE QSREC
    .     MUST BE CHANGED BY THE USER AS NECESSARY.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .**** THE FOLLOWING CARD IS RUN DEPENDENT.  IT SETS THE MAXIMUM TIME
    .**** ALLOWED FOR MODEL EXECUTION TO A NUMBER OF COMPUTING UNITS LESS
    .**** THAN THAT SPECIFIED ON THE JOBCARD.  THIS ALLOWS TIME FOR FILE
    .**** HANDLING IN CASE THE TIME LIMIT IS EXCEEDED.
(4) SCP, A=2600.
    DISKHOG, 10000.
    .
    .
    .... GET THE INPUT FILES FROM PSS AND MAGNETIC TAPE
    .**** THE FOLLOWING CARDS ARE RUN AND/OR USER DEPENDENT.  THE USER
    .**** MUST CHANGE THEM TO PROVIDE HIS OR HER OWN INPUT FILES.
    LIBCOPY, LIRAQ, QSRUN, QSRUN1.
    FETCHPS, MASCON, QGEO, QGEOSTL.
    GETTAPE, DAY76195/QICON, 16449.
    GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN0, 16449.
    GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN1, 16449.
    GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN2, 16449.
    GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN3, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN4, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN5, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN6, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN7, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN8, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN9, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRANA, 16449.
(5) .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRANB, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR00, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR01, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR02, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR03, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR04, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR05, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR06, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR07, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR08, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR09, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR10, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR11, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR12, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR13, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR14, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR15, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR16, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR17, 16449.
```

FIGURE J-6. Sample of LR1SLGO, the control card deck that executes LIRAQ-1S.

```
    GETTAPE, DAY76195/GS5KM/QSOR18, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR19, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR20, 16449.
(5) GETTAPE, DAY76195/GS5KM/QSOR21, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR22, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR23, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR24, 16449.
    .
    .
    .... LOAD AND EXECUTE
    FETCHPS, LIRAQ, LR1SBN, LR1SBN.
    GETTAPE, SCBN=GRAPHIC/SCLGOF, 16964, DATE=02DEC78.
    GETTAPE, ULIB=IDDSTST/ULIB, 16964, DATE=02DEC78.
    GETTAPE, TV80TLB=GRAPHICS/TV80TLB, 16964, DATE=02DEC78.
    LINK, F=LR1SBN, F=SCBN, L=0, P=ULIB, P=TV80TLB, RF, X.
    EXIT.
    DUMP, 0.
    FETCHPS, LIRAQ, LR1SSYM, LR1SSYM.
    GRUMP, P=LR1SSYM.
    REWIND, QSRUN.
    COPYSBF, QSRUN, OUTPUT.
    RETURN, QSRUN.
    CXIT.
    FIN.
    SFL, 50000,0.
    SCP, A=0.
    RETURN, DBGMAP, GRUMP.
    TIM.
    FILES.
    .
    .
    RENAME, TAPE3=QHSP.
    DISPOSE, QHSP=MF, T=[LIRAQ1S - QHSP].
    .**** THE FOLLOWING CARD IS RUN DEPENDENT.  THE TAPE NUMBER MUST BE
    .**** CHANGED TO SPECIFY A TAPE OWNED BY THE USER.
    RENAME, TAPE12=QSREC.
(6) .STOTAPE, DAY76195/INTERVAL3/GS5KM/RUN1001/QSREC, 13349.
    CXIT.
    EXIT.
    FIN.
    .
    .
    .... MICROFICHE ARCHIVE OF RUN WITH GRAPHICS
    TIM.
    DDB.
    REWIND, DAYFILE.
    FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
    FISHTLT, DAYFILE.
    RETURN, FISHTLT.
    TEXT, ARCHIVE, [$RU].
    TEXT, ARCHIVE, [$B=DAYFILE].
    COPY, DAYFILE/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=INPUT].
    REWIND, INPUT.
    COPYSBF, INPUT, ARCHIVE.
    DELETE, INPUT.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=QSRUN].
    REWIND, QSRUN.
    COPYSBF, QSRUN, ARCHIVE.
    RETURN, QSRUN.
```

FIGURE J-6. Continued.

TYPING GUIDE SHEET
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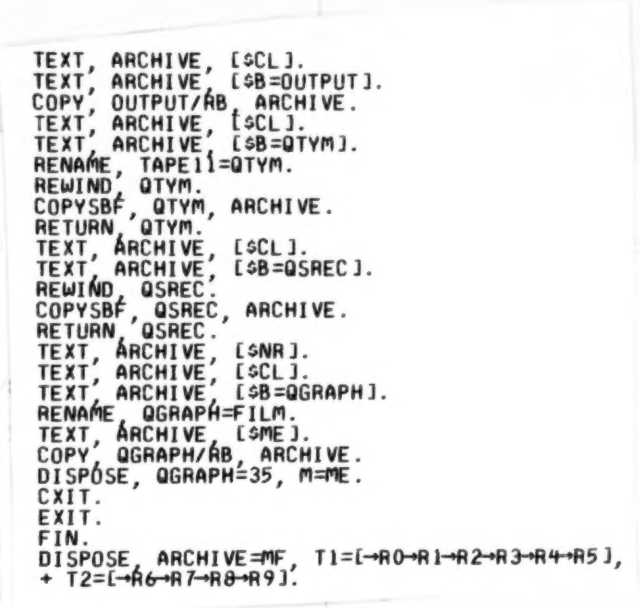

```
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=OUTPUT].
COPY, OUTPUT/RB, ARCHIVE.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QTYM].
RENAME, TAPE11=QTYM.
REWIND, QTYM.
COPYSBF, QTYM, ARCHIVE.
RETURN, QTYM.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QSREC].
REWIND, QSREC.
COPYSBF, QSREC, ARCHIVE.
RETURN, QSREC.
TEXT, ARCHIVE, [$NR].
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QGRAPH].
RENAME, QGRAPH=FILM.
TEXT, ARCHIVE, [$ME].
COPY, QGRAPH/RB, ARCHIVE.
DISPOSE, QGRAPH=35, M=ME.
CXIT.
EXIT.
FIN.
DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
+ T2=[→R6→R7→R8→R9].
```

FIGURE J-6. Continued.

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```
(1) LR2S,5,24000.679656,GRANT,K
    *HOLDOUT
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .# LIRAQ2S MCDEL EXECUTION DAY195 GS5KM INTERVAL3 NEW BC,IC
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .     THIS CONTROL DECK EXECUTES THE LIRAQ2S MODEL.  CONTROL CARDS TO
    .     OBTAIN THE INPUT FILES, QGEO AND QSRUN, TO OBTAIN THE QSOR AND
    .     QTRAN INPUT FILE FAMILIES, AND TO SAVE THE OUTPUT FILE QSREC
    .     MUST BE CHANGED BY THE USER AS NECESSARY.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .**** THE FOLLOWING CARD IS RUN DEPENDENT.  IT SETS THE MAXIMUM TIME
    .**** ALLOWED FOR MODEL EXECUTION TO A NUMBER OF COMPUTING UNITS LESS
    .**** THAN THAT SPECIFIED ON THE JOBCARD.  THIS ALLOWS TIME FOR FILE
    .**** HANDLING IN CASE THE TIME LIMIT IS EXCEEDED.
(4) SCP, A=22400.
    DISKHOG, 10000.
    .
    .
    .... GET THE INPUT FILES FROM PSS AND MAGNETIC TAPE
    .**** THE FOLLOWING CARDS ARE RUN AND/OR USER DEPENDENT.  THE USER
    .**** MUST CHANGE THEM TO PROVIDE HIS OR HER OWN INPUT FILES.
    LIBCOPY, LIRAQ, QSRUN, QSRUN2.
    FETCHPS, LIRAQ, QRAD, QRAD.
    FETCHPS, MASCON, QGEO, QGEOSTL.
    GETTAPE, DAY76195/QICON, 16449.
    GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN0, 16449.
    GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN1, 16449.
    GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN2, 16449.
    GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN3, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN4, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN5, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN6, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN7, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN8, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRAN9, 16449.
    .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRANA, 16449.
(5) .GETTAPE, DAY76195/INTERVAL3/GS5KM/QTRANB, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR00, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR01, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR02, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR03, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR04, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR05, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR06, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR07, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR08, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR09, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR10, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR11, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR12, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR13, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR14, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR15, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR16, 16449.
```

FIGURE J-7. Sample of LR2SLGO, the control card deck that executes LIRAQ-2S.

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```
    GETTAPE, DAY76195/GS5KM/QSOR17, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR18, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR19, 16449.
(5) GETTAPE, DAY76195/GS5KM/QSOR20, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR21, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR22, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR23, 16449.
    GETTAPE, DAY76195/GS5KM/QSOR24, 16449.
    .
    .
    .... LOAD AND EXECUTE
    FETCHPS, LIRAQ, LR2SBN, LR2SBN.
    GETTAPE, SCBN=GPACBN7/SCBN, 16964, DATE=15DEC78.
    GETTAPE, ULIB=IDDSTST/ULIBX, 16964, DATE=02DEC78.
    GETTAPE, TV80TLB=GRAPHICS/TV80TLB, 16964, DATE=02DEC78.
    LINK, F=LR2SBN, F=SCBN, L=0, P=ULIB, P=TV80TLB, RF, X.
    EXIT.
    DUMP, 0.
    FETCHPS, LIRAQ, LR2SSYM, LR2SSYM.
    GRUMP, P=LR2SSYM.
    REWIND, QSRUN.
    COPYSBF, QSRUN, OUTPUT.
    CXIT.
    FIN.
    SFL, 50000,0.
    SCP, A=0.
    RETURN, DBGMAP, GRUMP.
    TIM.
    FILES.
    .
    .
    RENAME, TAPE3=QHSP.
    DISPOSE, QHSP=MF, T=[LIRAQ2S - QHSP].
    .**** THE FOLLOWING CARD IS RUN DEPENDENT.  THE TAPE NUMBER MUST BE
    .**** CHANGED TO SPECIFY A TAPE OWNED BY THE USER.
    RENAME, TAPE12=QSREC.
    STOTAPE, DAY76195/INTERVAL3/GS5KM/RUN2003/QSREC, 13349.
(6) STOTAPE,DAY76195/INTERVAL3/GS5KM/RUN2003/QREST,13349.
    CXIT.
    EXIT.
    FIN.
    .
    .
    .... MICROFICHE ARCHIVE OF RUN WITH GRAPHICS
    TIM.
    DDB.
    REWIND, DAYFILE.
    FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
    FISHTLT, DAYFILE.
    RETURN, FISHTLT.
    TEXT, ARCHIVE, [$RU].
    TEXT, ARCHIVE, [$B=DAYFILE].
    COPY, DAYFILE/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=INPUT].
    REWIND, INPUT.
    COPYSBF, INPUT, ARCHIVE.
    DELETE, INPUT.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=QSRUN].
    REWIND, QSRUN.
    COPYSBF, QSRUN, ARCHIVE.
```

FIGURE J-7. Continued.

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```
RETURN, QSRUN.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=OUTPUT].
COPY, OUTPUT/RB, ARCHIVE.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QSTEP].
REWIND, QSTEP.
COPYSBF, QSTEP, ARCHIVE.
RETURN, QSTEP.
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QSREC].
REWIND, QSREC.
COPYSBF, QSREC, ARCHIVE.
RETURN, QSREC.
TEXT, ARCHIVE, [$NR].
TEXT, ARCHIVE, [$CL].
TEXT, ARCHIVE, [$B=QGRAPH].
RENAME, QGRAPH=FILM.
TEXT, ARCHIVE, [$ME].
COPY, QGRAPH/RB, ARCHIVE.
DISPOSE, QGRAPH=35, M=ME.
CXIT.
EXIT.
FIN.
DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
+ T2=[→R6→R7→R8→R9].
```

FIGURE J-7. Continued.

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5. Data Retrieval — The various LIBCOPY, FETCHPS and GETTAPE cards must be altered to retrieve the files you need from your archive. Remember to comment out any GETTAPE cards that refer to nonexistent QTRANx or QSORxx files.

6. Data Storage — The STOTAPE address must be altered to reflect your archive structure.

Figure J-8 gives a sample of VERFLGO, the control card deck that executes VERF, the routine that compares model with observation. The indicated 7 cards must be modified:

1. Job Card — The job card must be given your name and valid LBL account number.

2. Routing Information — The routing instructions must be include your address.

3. Title Card — The title should be whatever you want.

4. The QSREC and QICON file you wish to compare must be retrieved from your archive.

5. Either a blank card (for St. Louis) or any number (for San Francisco) must be entered in columns 6-15 of the first card after the end of record card.

6. The pollutants of interest must be given (in 6I2 format) or the second card after the end of record card. Here 1=carbon monoxide, 2=hydrocarbons, 3=nitric oxide, 4=nitrogen dioxide, 5=ozone, and 6=sulphur dioxide.

7. The third card after the end of record card must contain the hours (local standard time) for which the data are to be compared. The format is 2F5.2, and the hours requested must be included in both QSREC and QICON.

The following decks are designed to recompile the various routines associated with the LIRAQ models. The user should only use these decks if he is satisfied that he understands both the processor coding and the UPDATE process. Before changing any of the compiled codes in the data cell libraries, MASCON, LIRAQ, LIRVERF, EPA or VERF, please clear the changes with W. H. Duewer, L-262, Lawrence Livermore Laboratory, Phone: 415-422-1807 (FTS: 532-1807). If you wish to recompile the codes and store the compiled codes in your own archive that is your privilege. However, if you do so, you will need to alter the decks that execute the various codes so that they retrieve the binary files from your archive rather than ours.

Figure J-9 lists a sample SPRCCD, the control card deck that compiles the source processor. There are four portions of this deck that must be modified for a recompilation.

1. Job Card — The job card must be modified to have your name and your account.

2. Routing Information — The routine instructions must have your address.

```
(1)  VERF,07,300.679656,GRANT,K
     *HOLDOUT
(2)  (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3)  .≠ VERF MODEL/OBSERVATIONS PLOTS
     ..
     .. FETCH INPUT FILES
(4)  GETTAPE, DAY76196/INTERVAL3/GS5KM/RUN1001/QSREC,13349.
     GETTAPE, DAY76196/QICON,16449.
     ..
     .. LOAD AND EXECUTE
     FETCHPS, LIRVERF, LGO, VERFBN.
     GETTAPE, SCLGOF=GRAPHIC/SCLGOF, 16964, DATE=02DEC78.
     GETTAPE, ULIB=IDDSTST/ULIB, 16964, DATE=02DEC78.
     LINK, F, F=SCLGOF, L=0, P=ULIB, RF, X.
     CXIT.
     END.
     EXIT.
     END.
     FIN.
     ..
     .. CREATE ARCHIVE FILE
     TEXT, ARCHIVE, [$RU].
     TEXT, ARCHIVE, [$B=DAYFILE].
     TIM.
     DDB.
     FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
     REWIND, DAYFILE.
     FISHTLT, DAYFILE.
     RETURN, FISHTLT.
     COPY, DAYFILE/RX, ARCHIVE.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=INPUT].
     REWIND, INPUT.
     COPYSBF, INPUT, ARCHIVE.
     RETURN, INPUT.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=QSREC].
     REWIND, QSREC.
     COPYSBF, QSREC, ARCHIVE.
     RETURN, QSREC.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=QICON].
     REWIND, QICON.
     COPYSBF, QICON, ARCHIVE.
     RETURN, QICON.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=OUTPUT].
     COPY, OUTPUT/RB, ARCHIVE.
     DELETE, OUTPUT.
     TEXT, ARCHIVE, [$NR].
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=GRAPHS].
     TEXT, ARCHIVE, [$ME].
     COPY, FILM/RB, ARCHIVE.
     DISPOSE, FILM=35, M=ME.
     DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
     + T2=[→R6→R7→R8→R9].
(5)    196             ANY NUMBER IN COL'S 6-15 GIVES SF FORMAT.  BLANK GIVES SL
(6)   1 2 3 4 5 6 6I2 FORMAT SPECIFIES POLLUTANTS
(7)   0.0  20.0    2F5.2 SPECIFIES TIME WINDOW
```

FIGURE J-8. Sample of VERFLGO, the control card deck that executes VERF.

```
(1) SPRC,7,500.679656,GRANT,K
    *HOLDOUT
    *PSS
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .# SORPROC UPDATE AND COMPILATION
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE UPDATE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .  AVAILABILITY...
    .        THIS CONTROL DECK MAY BE OBTAINED BY EXECUTING THE CONTROL
    .        CARD
    .           FETCHPS, SORPROC, SPRCCD, SPRCCD.
    .
    .  PURPOSE...
    .        THIS DECK PERFORMS THE FOLLOWING TASKS -
    .           1) UPDATES THE SOURCE PROCESSOR (SORPROC) PROGRAM LIBRARY
    .              'SPRCPL' FROM DIRECTIVES ON THE FILE 'SPMOD'.
    .           2) GENERATES A RELOCATABLE BINARY FILE 'SPRCBN'
    .           3) GENERATES A GRUMP SYMBOL TABLE FILE 'SPRCSYM'
    .
    .        THE FILE 'SPMOD' CONTAINS THE MODIFICATIONS TO BE MADE TO
    .        'SPRCPL'.  AS EACH 'SPMOD' DECK IS RUN, IT SHOULD BE ARCHIVED
    .        TO A PSS SUBSET WHOSE NAME IS OF THE FORM 'SPYMMDD', WHERE
    .        DD=DAY, MM=MONTH, AND Y=LAST DIGIT OF THE YEAR.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .
    DISKHOG, 20000.
    FETCHPS, SORPROC, OLDPL, SPRCPL.
    .**** THE FOLLOWING CARD IS UPDATE DEPENDENT.  MAKE SURE THAT IT
    .**** FETCHES THE LATEST UPDATE WHICH IS TO BE APPLIED TO THE SORPROC
    .**** PROGRAM LIBRARY.
(4) LIBCOPY, SORPROC, SPMOD, SP00000.
    .
    .
    ..... GENERATE THE COMPILE FILE AND CREATE A NEW PROGRAM LIBRARY
    TEXT, LIST, [$B=UPDATE].
    UPDATE, F, I=SPMOD, LC=10000, N=SPRCPL, O=LIST.
    RETURN, SPMOD, OLDPL.
    FTN4, B=SPRCBN, I=COMPILE, L=COMP, LCM=I, OPT=2, R=3.
    EXIT.
    COPY, COMP/RR, LIST.
    BGNSKIP.
    FIN.
    RETURN, COMPILE.
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=COMPILE].
    COPY, COMP/RR, LIST.
    .
    .
    ..... TEST LOAD THE NEW BINARY FILE
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=LOADMAP].
    LINK, F=SPRCBN, L=LIST, LO=BERX.
    SFL, 50000,0.
    .
    .
```

FIGURE J-9. Sample of SPRCCD, the control card deck that compiles the source processor.

```
      ..... GENERATE THE SYMBOL TABLE
      GRUMP, L=0, P=COMP, WSYM=SPRCSYM.
      RETURN, COMP.
      REWIND, SPRCBN.
      SYMLIST, SPRCBN, SYM.
      .
      .
      ..... NO ERRORS - UPDATE SORPROC ON PSS
      TEXT, TEMP, [GROUP = 227, GDIV].
      TEXT, TEMP, [OWNER = GRANT,K].
      TEXT, TEMP, [CHANGE LIBRARY = SORPROC].
      TEXT, TEMP, [DESTROY SUBSET = SPRCPLO].
      TEXT, TEMP, [RENAME SUBSET SPRCPL=SPRCPLO].
      TEXT, TEMP, [CREATE SUBSET = SPRCPL].
(5)   TEXT, TEMP, [COPY 0 F FROM FILE = SPRCPL].
      TEXT, TEMP, [REPLACE SUBSET = SPRCBN].
      TEXT, TEMP, [COPY 0 F FROM FILE = SPRCBN].
      TEXT, TEMP, [REPLACE SUBSET = SPRCSYM].
      TEXT, TEMP, [COPY 0 F FROM FILE = SPRCSYM].
      TEXT, TEMP, [END].
      COPY, TEMP/RX, OFXB, CPSSIN/RR.
      .
      COPYPSS, CPSSIN.
      RETURN, CPSSIN.
      ENTERPS, SORPROC, SPRCPL, SPRCPL.
      ENTERPS, SORPROC, SPRCBN, SPRCBN.
      ENTERPS, SORPROC, SPRCSYM, SPRCSYM.
      .
      .
      ..... CREATE AN ARCHIVE FILE OF THIS SORPROC UPDATE FOR OUTPUT
      ..... AS MICROFICHE.
      EXIT.
      CXIT.
      FIN.
      ENDSKIP.
      SFL, 50000, 0.
      TIM.
      DDB.
      FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
      REWIND, DAYFILE.
      FISHTLT, DAYFILE.
      TEXT, ARCHIVE, [$RU].
      TEXT, ARCHIVE, [$B=DAYFILE].
      COPY, DAYFILE/RX, ARCHIVE.
      TEXT, ARCHIVE, [$CL].
      TEXT, ARCHIVE, [$B=INPUT].
      REWIND, INPUT.
      COPYSBF, INPUT, ARCHIVE.
      RETURN, INPUT.
      TEXT, ARCHIVE, [$CL].
      TEXT, ARCHIVE, [$B=OUTPUT].
      COPY, OUTPUT/RR, ARCHIVE.
      TEXT, ARCHIVE, [$CL].
      COPY, LIST/RX, ARCHIVE.
      TEXT, ARCHIVE, [$CL].
      TEXT, ARCHIVE, [$B=SYMLIST].
      COPY, SYM/RX, ARCHIVE.
      DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
      +T2=[→R6→R7→R8→R9].
```

FIGURE J-9. Continued.

3. Title Card — The title should be whatever you want.

4. The LIBCOPY card that accesses your UPDATE deck must be modified to fetch your valid FTN update deck from your directory. See an FTN manual for instructions.

5. Data Storage — The storage instructions for the output must be modified to be compatible with your archive.

Figure J-10 lists a sample RDARCD, the control card deck that compiles RDAR, a data format converter called by SPRCLGO. The same five items must be altered in RDARCD as in SPRCCD.

Figure J-11 lists a sample RDPTCD, the control card deck that compiles RDPT, a data format converter called by SPRCLGO. See the discussion of SPRCCD for a list of commands to be modified.

Figure J-12 lists a sample QPRCCD, the deck that compiles the Q-Processor. The following cards should be modified before executing QPRCCD.

1. Job Card — The job card should have your name and LBL account number.
2. Routing Information — The routine instructions should have your address.
3. Title Card — The title should be whatever you want.
4. The LIBCOPY card should fetch a QPMOD deck that serves as a valid FTN UPDATE deck.
5. Data Storage — The routing of the compiler output should be altered to send the data to the appropriate archive.

Figure J-13 gives a sample MPRCCD, the deck that compiles the M-Processor. The following cards should be modified prior to executing MPRCCD.

1. Job Card — The job card should contain your name and LBL account number.
2. Routing Information — The routing instructions should give your address.
3. Title Card — The title should be whatever you want.
4. Data Retrieval — The LIBCOPY that retrieves MPMOD should recover your valid FTN UPDATE deck.
5. Data Storage — The compiled files should be routed to the appropriate archive.

Figure J-14 gives a sample of MSCNCD, the deck that compiles MASCON. Before executing MSCNCD the following cards should be modified:

```
(1) RDAR,7,100.679656,GRANT,K
    *HOLDOUT
    *PSS
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .≠ READAR UPDATE AND COMPILATION
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE UPDATE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .  AVAILABILITY...
    .        THIS CONTROL DECK MAY BE OBTAINED BY EXECUTING THE CONTROL
    .        CARD
    .           FETCHPS, SORPROC, RDARCD, RDARCD.
    .
    .  PURPOSE...
    .        THIS DECK PERFORMS THE FOLLOWING TASKS -
    .           1) UPDATES THE READAR PROGRAM LIBRARY 'RDARPL' FROM
    .              DIRECTIVES ON THE FILE 'ARMOD'.
    .           2) GENERATES A RELOCATABLE BINARY FILE 'RDARBN'
    .           3) GENERATES A GRUMP SYMBOL TABLE FILE 'RDARSYM'
    .
    .        THE FILE 'ARMOD' CONTAINS THE MODIFICATIONS TO BE MADE TO
    .        'RDARPL'.  AS EACH 'ARMOD' DECK IS RUN, IT SHOULD BE ARCHIVED
    .        TO A PSS SUBSET WHOSE NAME IS OF THE FORM 'ARYMMDD', WHERE
    .        DD=DAY, MM=MONTH, AND Y=LAST DIGIT OF THE YEAR.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .
    DISKHOG, 20000.
    FETCHPS, SORPROC, OLDPL, RDARPL.
    .**** THE FOLLOWING CARD IS UPDATE DEPENDENT.  MAKE SURE THAT IT
    .**** FETCHES THE LATEST UPDATE WHICH IS TO BE APPLIED TO THE READAR
    .**** PROGRAM LIBRARY.
(4) LIBCOPY, SORPROC, ARMOD, AR00000.
    .
    .
    ..... GENERATE THE COMPILE FILE AND CREATE A NEW PROGRAM LIBRARY
    TEXT, LIST, [$B=UPDATE].
    UPDATE, F, I=ARMOD, LC=10000, N=RDARPL, O=LIST.
    RETURN, ARMOD, OLDPL.
    FTN4, B=RDARBN, I=COMPILE, L=COMP, LCM=I, OPT=2, R=3.
    CXIT.
    COPY, COMP/RR, LIST.
    BGNSKIP.
    FIN.
    RETURN, COMPILE.
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=COMPILE].
    COPY, COMP/RR, LIST.
    .
    .
    ..... TEST LOAD THE NEW BINARY FILE
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=LOADMAP].
    LINK, F=RDARBN, L=LIST, LO=BERX.
    SFL, 50000,0.
    .
    .
```

FIGURE J-10. Example of RDARCD, the control card deck that compiles RDAR.

```
     ..... GENERATE THE SYMBOL TABLE
     GRUMP, L=0, P=COMP, WSYM=RDARSYM.
     RETURN, COMP.
     REWIND, RDARBN.
     SYMLIST, RDARBN, SYM.
     .
     .
     ..... NO ERRORS - UPDATE READAR ON PSS
     TEXT, TEMP, [GROUP = 227, GDIV].
     TEXT, TEMP, [OWNER = GRANT,K].
     TEXT, TEMP, [CHANGE LIBRARY = SORPROC].
     TEXT, TEMP, [DESTROY SUBSET = RDARPLO].
     TEXT, TEMP, [RENAME SUBSET RDARPL=RDARPLO].
(5)  TEXT, TEMP, [CREATE SUBSET = RDARPL].
     TEXT, TEMP, [COPY 0 F FROM FILE = RDARPL].
     TEXT, TEMP, [REPLACE SUBSET = RDARBN].
     TEXT, TEMP, [COPY 0 F FROM FILE = RDARBN].
     TEXT, TEMP, [REPLACE SUBSET = RDARSYM].
     TEXT, TEMP, [COPY 0 F FROM FILE = RDARSYM].
     TEXT, TEMP, [END].
     COPY, TEMP/RX, OFXB, CPSSIN/RR.
     .
     COPYPSS, CPSSIN.
     RETURN, CPSSIN.
     ENTERPS, SORPROC, RDARPL, RDARPL.
     ENTERPS, SORPROC, RDARBN, RDARBN.
     ENTERPS, SORPROC, RDARSYM, RDARSYM.
     .
     .
     ..... CREATE AN ARCHIVE FILE OF THIS READAR UPDATE FOR OUTPUT
     ..... AS MICROFICHE.
     EXIT.
     CXIT.
     FIN.
     ENDSKIP.
     SFL, 50000, 0.
     TIM.
     DDB.
     FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
     REWIND, DAYFILE.
     FISHTLT, DAYFILE.
     TEXT, ARCHIVE, [$RU].
     TEXT, ARCHIVE, [$B=DAYFILE].
     COPY, DAYFILE/RX, ARCHIVE.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=INPUT].
     REWIND, INPUT.
     COPYSBF, INPUT, ARCHIVE.
     RETURN, INPUT.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=OUTPUT].
     COPY, OUTPUT/RR, ARCHIVE.
     TEXT, ARCHIVE, [$CL].
     COPY, LIST/RX, ARCHIVE.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=SYMLIST].
     COPY, SYM/RX, ARCHIVE.
     DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
     +T2=[→R6→R7→R8→R9].
```

FIGURE J-10. Continued.

```
(1) RDPT,7,100.679656,GRANT,K
    *HOLDOUT
    *PSS
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .≠ READPT UPDATE AND COMPILATION
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE UPDATE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .  AVAILABILITY...
    .        THIS CONTROL DECK MAY BE OBTAINED BY EXECUTING THE CONTROL
    .        CARD
    .           FETCHPS, SORPROC, RDPTCD, RDPTCD.
    .
    .  PURPOSE...
    .        THIS DECK PERFORMS THE FOLLOWING TASKS -
    .           1) UPDATES THE READPT PROGRAM LIBRARY 'RDPTPL' FROM
    .              DIRECTIVES ON THE FILE 'PTMOD'.
    .           2) GENERATES A RELOCATABLE BINARY FILE 'RDPTBN'
    .           3) GENERATES A GRUMP SYMBOL TABLE FILE 'RDPTSYM'
    .
    .        THE FILE 'PTMOD' CONTAINS THE MODIFICATIONS TO BE MADE TO
    .        'RDPTPL'.  AS EACH 'PTMOD' DECK IS RUN, IT SHOULD BE ARCHIVED
    .        TO A PSS SUBSET WHOSE NAME IS OF THE FORM 'PTYMMDD', WHERE
    .        DD=DAY, MM=MONTH, AND Y=LAST DIGIT OF THE YEAR.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .
    DISKHOG, 20000.
    FETCHPS, SORPROC, OLDPL, RDPTPL.
    .**** THE FOLLOWING CARD IS UPDATE DEPENDENT.  MAKE SURE THAT IT
    .**** FETCHES THE LATEST UPDATE WHICH IS TO BE APPLIED TO THE READPT
    .**** PROGRAM LIBRARY.
(4) LIBCOPY, SORPROC, PTMOD, PT00000.
    .
    .
    ..... GENERATE THE COMPILE FILE AND CREATE A NEW PROGRAM LIBRARY
    TEXT, LIST, [$B=UPDATE].
    UPDATE, F, I=PTMOD, LC=10000, N=RDPTPL, O=LIST.
    RETURN, PTMOD, OLDPL.
    FTN4, B=RDPTBN, I=COMPILE, L=COMP, LCM=I, OPT=2, R=3.
    CXIT.
    COPY, COMP/RR, LIST.
    BGNSKIP.
    FIN.
    RETURN, COMPILE.
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=COMPILE].
    COPY, COMP/RR, LIST.
    .
    .
    ..... TEST LOAD THE NEW BINARY FILE
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=LOADMAP].
    LINK, F=RDPTBN, L=LIST, LO=BERX.
    SFL, 50000,0.
    .
    .
```

FIGURE J-11. Sample of RDPTCD, the control card deck that recompiles RDPT.

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TYPING GUIDE SHEET
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TOP OF IMAGE AREA
DROPPED HEAD BEGIN FIRST LINE HERE
BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
BEGIN LAST LINE OF TEXT
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TYPING GUIDE SHEET
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TOP OF IMAGE AREA
BEGIN FIRST LINE OF TEXT HERE

```
    ..... GENERATE THE SYMBOL TABLE
    CRUMP, L=0, P=COMP, WSYM=RDPTSYM.
    RETURN, COMP.
    REWIND, RDPTBN.
    SYMLIST, RDPTBN, SYM.
    .
    .
    ..... NO ERRORS - UPDATE READPT ON PSS
    TEXT, TEMP, [GROUP = 227, GDIV].
    TEXT, TEMP, [OWNER = GRANT,K].
    TEXT, TEMP, [CHANGE LIBRARY = SORPROC].
    TEXT, TEMP, [DESTROY SUBSET = RDPTPLO].
    TEXT, TEMP, [RENAME SUBSET RDPTPL=RDPTPLO].
    TEXT, TEMP, [CREATE SUBSET = RDPTPL].
(5) TEXT, TEMP, [COPY 0 F FROM FILE = RDPTPL].
    TEXT, TEMP, [REPLACE SUBSET = RDPTBN].
    TEXT, TEMP, [COPY 0 F FROM FILE = RDPTBN].
    TEXT, TEMP, [REPLACE SUBSET = RDPTSYM].
    TEXT, TEMP, [COPY 0 F FROM FILE = RDPTSYM].
    TEXT, TEMP, [END].
    COPY, TEMP/RX, OFXB, CPSSIN/RR.
    .
    COPYPSS, CPSSIN.
    RETURN, CPSSIN.
    ENTERPS, SORPROC, RDPTPL, RDPTPL.
    ENTERPS, SORPROC, RDPTBN, RDPTBN.
    ENTERPS, SORPROC, RDPTSYM, RDPTSYM.
    .
    .
    ..... CREATE AN ARCHIVE FILE OF THIS READPT UPDATE FOR OUTPUT
    ..... AS MICROFICHE.
    EXIT.
    CXIT.
    FIN.
    ENDSKIP.
    SFL, 50000, 0.
    TIM.
    DDB.
    FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
    REWIND, DAYFILE.
    FISHTLT, DAYFILE.
    TEXT, ARCHIVE, [$RU].
    TEXT, ARCHIVE, [$B=DAYFILE].
    COPY, DAYFILE/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=INPUT].
    REWIND, INPUT.
    COPYSBF, INPUT, ARCHIVE.
    RETURN, INPUT.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=OUTPUT].
    COPY, OUTPUT/RR, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    COPY, LIST/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=SYMLIST].
    COPY, SYM/RX, ARCHIVE.
    DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
    +T2=[→R6→R7→R8→R9].
```

FIGURE J-11. Continued.

BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
BEGIN LAST LINE OF TEXT
3/8"

PAGE NUMBER
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(4-76)

```
(1) QPRC,7.679656,GRANT,K
    *HOLDOUT
    *PSS
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .# Q-PROCESSOR UPDATE AND COMPILATION
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE UPDATE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .  AVAILABILITY...
    .        THIS CONTROL DECK MAY BE OBTAINED BY EXECUTING THE CONTROL
    .        CARD
    .           FETCHPS, MASCON, QPRCCD, QPRCCD.
    .
    .  PURPOSE...
    .        THIS DECK PERFORMS THE FOLLOWING TASKS -
    .           1) UPDATES THE Q-PROCESSOR (Q-PROC) PROGRAM LIBRARY
    .              'QPRCPL' FROM DIRECTIVES ON THE FILE 'QPMOD'.
    .           2) GENERATES A RELOCATABLE BINARY FILE 'QPRCBN'
    .
    .        THE FILE 'QPMOD' CONTAINS THE MODIFICATIONS TO BE MADE TO
    .        'QPRCPL'.  AS EACH 'QPMOD' DECK IS RUN, IT SHOULD BE ARCHIVED
    .        TO A PSS SUBSET WHOSE NAME IS OF THE FORM 'QPYMMDD', WHERE
    .        DD=DAY, MM=MONTH, AND Y=LAST DIGIT OF THE YEAR.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .
    FETCHPS, MASCON, OLDPL, QPRCPL.
    .**** THE FOLLOWING CARD IS UPDATE DEPENDENT.  MAKE SURE THAT IT
    .**** FETCHES THE LATEST UPDATE WHICH IS TO BE APPLIED TO THE Q-PROC
    .**** PROGRAM LIBRARY.
(4) LIBCOPY, MASCON, QPMOD, QP00000.
    .
    .
    ..... GENERATE THE COMPILE FILE AND CREATE A NEW PROGRAM LIBRARY
    TEXT, LIST, [$B=UPDATE].
    UPDATE, F, I=QPMOD, LC=10000, N=QPRCPL, O=LIST.
    RETURN, QPMOD, OLDPL.
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=COMPILE].
    FETCHPS, PASCAL, PASCAL, PASCAL.
    SFL, 100000.
    PASCAL, COMPILE, LIST, QPRCBN.
    RETURN, COMPILE, PASCAL.
    CXIT.
    RETURN, COMPILE, PASCAL.
    BGNSKIP.
    FIN.
    RETURN, COMPILE.
    .
    .
    ..... TEST LOAD THE NEW BINARY FILE
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=LOADMAP].
    FETCHPS, PASCAL, PASLIB, PASLIB.
    LINK, F=QPRCBN, FL=0, L=LIST, LO=BERX, P=PASLIB.
    RETURN, PASLIB.
    SFL, 50000,0.
```

FIGURE J-12. Sample of QPRCCD, the control card deck that recompiles the Q-processor.

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD: BEGIN SECTIONS HERE

```
       .
       .
       ..... GENERATE THE SYMBOL TABLE
       REWIND, QPRCBN.
       SYMLIST, QPRCBN, SYM.
       .
       .
      [..... NO ERRORS - UPDATE Q-PROC ON PSS
      |TEXT, TEMP, [GROUP = 227, GDIV].
      |TEXT, TEMP, [OWNER = GRANT,K].
      |TEXT, TEMP, [CHANGE LIBRARY = MASCON].
      |TEXT, TEMP, [DESTROY SUBSET = QPRCPLO].
      |TEXT, TEMP, [RENAME SUBSET QPRCPL=QPRCPLO].
  (5) |TEXT, TEMP, [CREATE SUBSET = QPRCPL].
      |TEXT, TEMP, [COPY 0 F FROM FILE = QPRCPL].
      |TEXT, TEMP, [REPLACE SUBSET = QPRCBN].
      |TEXT, TEMP, [COPY 0 F FROM FILE = QPRCBN].
      |TEXT, TEMP, [END].
      |COPY, TEMP/RX, OFXB, CPSSIN/RR.
      L.
       COPYPSS, CPSSIN.
       RETURN, CPSSIN.
       ENTERPS, MASCON, QPRCPL, QPRCPL.
       ENTERPS, MASCON, QPRCBN, QPRCBN.
       .
       .
       ..... CREATE AN ARCHIVE FILE OF THIS Q-PROC UPDATE FOR OUTPUT
       ..... AS MICROFICHE.
       EXIT.
       CXIT.
       FIN.
       ENDSKIP.
       SFL, 50000, 0.
       TIM.
       DDB.
       FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
       REWIND, DAYFILE.
       FISHTLT, DAYFILE.
       TEXT, ARCHIVE, [$RU].
       TEXT, ARCHIVE, [$B=DAYFILE].
       COPY, DAYFILE/RX, ARCHIVE.
       TEXT, ARCHIVE, [$CL].
       TEXT, ARCHIVE, [$B=INPUT].
       REWIND, INPUT.
       COPYSBF, INPUT, ARCHIVE.
       RETURN, INPUT.
       TEXT, ARCHIVE, [$CL].
       TEXT, ARCHIVE, [$B=OUTPUT].
       COPY, OUTPUT/RR, ARCHIVE.
       TEXT, ARCHIVE, [$CL].
       COPY, LIST/RX, ARCHIVE.
       TEXT, ARCHIVE, [$CL].
       TEXT, ARCHIVE, [$B=SYMLIST].
       COPY, SYM/RX, ARCHIVE.
       DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
       +T2=[→R6→R7→R8→R9].
```

FIGURE J-12. Continued.

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BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"
PAGE NUMBER
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```
(1) MPRC,7.679656,GRANT,K
    *HOLDOUT
    *PSS
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .≠ M-PROCESSOR UPDATE AND COMPILATION
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE UPDATE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .  AVAILABILITY...
    .        THIS CONTROL DECK MAY BE OBTAINED BY EXECUTING THE CONTROL
    .        CARD
    .           FETCHPS, MASCON, MPRCCD, MPRCCD.
    .
    .  PURPOSE...
    .        THIS DECK PERFORMS THE FOLLOWING TASKS -
    .           1) UPDATES THE M-PROCESSOR (M-PROC) PROGRAM LIBRARY
    .              'MPRCPL' FROM DIRECTIVES ON THE FILE 'MPMOD'.
    .           2) GENERATES A RELOCATABLE BINARY FILE 'MPRCBN'
    .           3) GENERATES A GRUMP SYMBOL TABLE FILE 'MPRCSYM'
    .
    .        THE FILE 'MPMOD' CONTAINS THE MODIFICATIONS TO BE MADE TO
    .        'MPRCPL'.  AS EACH 'MPMOD' DECK IS RUN, IT SHOULD BE ARCHIVED
    .        TO A PSS SUBSET WHOSE NAME IS OF THE FORM 'MPYMMDD', WHERE
    .        DD=DAY, MM=MONTH, AND Y=LAST DIGIT OF THE YEAR.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .
    FETCHPS, MASCON, OLDPL, MPRCPL.
    .**** THE FOLLOWING CARD IS UPDATE DEPENDENT.  MAKE SURE THAT IT
    .**** FETCHES THE LATEST UPDATE WHICH IS TO BE APPLIED TO THE M-PROC
    .**** PROGRAM LIBRARY.
(4) LIBCOPY, MASCON, MPMOD, MP00000.
    .
    .
    ..... GENERATE THE COMPILE FILE AND CREATE A NEW PROGRAM LIBRARY
    TEXT, LIST, [$B=UPDATE].
    UPDATE, F, I=MPMOD, LC=10000, N=MPRCPL, O=LIST.
    RETURN, MPMOD, OLDPL.
    FTN4, B=MPRCBN, I=COMPILE, L=COMP, LCM=I, OPT=2, R=3.
    CXIT.
    COPY, COMP/RR, LIST.
    BGNSKIP.
    FIN.
    RETURN, COMPILE.
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=COMPILE].
    COPY, COMP/RR, LIST.
    .
    .
    ..... TEST LOAD THE NEW BINARY FILE
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=LOADMAP].
    LINK, F=MPRCBN, L=LIST, LO=BERX.
    SFL, 50000,0.
    .
    .
    ..... GENERATE THE SYMBOL TABLE
```

FIGURE J-13. Sample of MPRCCD, the control card deck that recompiles the M-processor.

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD BEGIN SECTIONS HERE

```
     GRUMP, L=0, P=COMP, WSYM=MPRCSYM.
     RETURN, COMP.
     REWIND, MPRCBN.
     SYMLIST, MPRCBN, SYM.
     .
     .
    ..... NO ERRORS - UPDATE M-PROC ON PSS
    TEXT, TEMP, [GROUP = 227, GDIV].
    TEXT, TEMP, [OWNER = GRANT,K].
    TEXT, TEMP, [CHANGE LIBRARY = MASCON].
    TEXT, TEMP, [DESTROY SUBSET = MPRCPLO].
    TEXT, TEMP, [RENAME SUBSET MPRCPL=MPRCPLO].
    TEXT, TEMP, [CREATE SUBSET = MPRCPL].
(5) TEXT, TEMP, [COPY 0 F FROM FILE = MPRCPL].
    TEXT, TEMP, [REPLACE SUBSET = MPRCBN].
    TEXT, TEMP, [COPY 0 F FROM FILE = MPRCBN].
    TEXT, TEMP, [REPLACE SUBSET = MPRCSYM].
    TEXT, TEMP, [COPY 0 F FROM FILE = MPRCSYM].
    TEXT, TEMP, [END].
    COPY, TEMP/RX, OFXB, CPSSIN/RR.
     .
     COPYPSS, CPSSIN.
     RETURN, CPSSIN.
     ENTERPS, MASCON, MPRCPL, MPRCPL.
     ENTERPS, MASCON, MPRCBN, MPRCBN.
     ENTERPS, MASCON, MPRCSYM, MPRCSYM.
     .
     .
     ..... CREATE AN ARCHIVE FILE OF THIS M-PROC UPDATE FOR OUTPUT
     ..... AS MICROFICHE.
     EXIT.
     CXIT.
     FIN.
     ENDSKIP.
     SFL, 50000, 0.
     TIM.
     DDB.
     FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
     REWIND, DAYFILE.
     FISHTLT, DAYFILE.
     TEXT, ARCHIVE, [$RU].
     TEXT, ARCHIVE, [$B=DAYFILE].
     COPY, DAYFILE/RX, ARCHIVE.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=INPUT].
     REWIND, INPUT.
     COPYSBF, INPUT, ARCHIVE.
     RETURN, INPUT.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=OUTPUT].
     COPY, OUTPUT/RR, ARCHIVE.
     TEXT, ARCHIVE, [$CL].
     COPY, LIST/RX, ARCHIVE.
     TEXT, ARCHIVE, [$CL].
     TEXT, ARCHIVE, [$B=SYMLIST].
     COPY, SYM/RX, ARCHIVE.
     DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
     +T2=[→R6→R7→R8→R9].
```

FIGURE J-13. Continued.

BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
BEGIN LAST LINE OF TEXT
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```
(1)  MSCN,7,500.679656,GRANT,K
     *HOLDOUT
     *PSS
(2)  (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3)  .# MASCON UPDATE AND COMPILATION
     .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
     .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
     .**** CARD CONTAINS THE UPDATE TITLE FOR LABELING OF JOB OUTPUT.
     .
     .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
     .
     .  AVAILABILITY...
     .        THIS CONTROL DECK MAY BE OBTAINED BY EXECUTING THE CONTROL
     .        CARD
     .           FETCHPS, MASCON, MSCNCD MSCNCD.
     .
     .  PURPOSE...
     .        THIS DECK PERFORMS THE FOLLOWING TASKS -
     .           1) UPDATES THE MASCON PROGRAM LIBRARY 'MSCNPL' FROM
     .              DIRECTIVES ON THE FILE 'LMOD'.
     .           2) GENERATES A RELOCATABLE BINARY FILE 'MSCNBN'
     .           3) GENERATES A GRUMP SYMBOL TABLE FILE 'MSCNSYM'
     .
     .        THE FILE 'LMOD' CONTAINS THE MODIFICATIONS TO BE MADE TO
     .        'MSCNPL'.  AS EACH 'LMOD' DECK IS RUN, IT SHOULD BE ARCHIVED
     .        TO A PSS SUBSET WHOSE NAME IS OF THE FORM 'LYMMDD', WHERE
     .        DD=DAY, MM=MONTH, AND Y=LAST DIGIT OF THE YEAR.
     .
     .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
     .
     .
     DISKHOG, 20000.
     FETCHPS, MASCON, OLDPL, MSCNPL.
     .**** THE FOLLOWING CARD IS UPDATE DEPENDENT.  MAKE SURE THAT IT
     .**** FETCHES THE LATEST UPDATE WHICH IS TO BE APPLIED TO THE MASCON
     .**** PROGRAM LIBRARY.
(4)  LIBCOPY, MASCON, LMOD, L00000.
     .
     .
     ..... GENERATE THE COMPILE FILE AND CREATE A NEW PROGRAM LIBRARY
     TEXT, LIST, [$B=UPDATE].
     UPDATE, F, I=LMOD, LC=10000, N=MSCNPL, O=LIST.
     RETURN, LMOD, OLDPL.
     TEXT, LIST, [$CL].
     TEXT, LIST, [$B=COMPILE].
     SFL, 100000,60000.
     FTN4, B=MSCNBN, I=COMPILE, L=COMP, LCM=I, OPT=2, R=3.
     CXIT.
     RETURN, COMPILE.
     COPY, COMP/RR, LIST.
     BGNSKIP.
     FIN.
     SFL, 50000,0.
     RETURN, COMPILE.
     COPY, COMP/RR, LIST.
     .
     .
     ..... TEST LOAD THE NEW BINARY FILE
     GETTAPE, ULIB=IDDSTST/ULIB, 16964, DATE=02DEC78.
     GETTAPE, SCLGOF=GRAPHIC/SCLGOF, 16964, DATE=02DEC78.
     GETTAPE, TV80TLB=GRAPHICS/TV80TLB, 16964, DATE=02DEC78.
```

FIGURE J-14. Sample of MSCNCD, the control card deck that recompiles MASCON.

```
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=LOADMAP].
    LINK, F=MSCNBN, F=SCLGOF, L=LIST, LO=BERX, P=ULIB, P=TV80TLB.
    SFL, 50000,0.
     .
     .
    ..... GENERATE THE SYMBOL TABLE
    GRUMP, L=0, P=COMP, WSYM=MSCNSYM.
    RETURN, COMP.
    REWIND, MSCNBN.
    SYMLIST, MSCNBN, SYM.
     .
     .
    ..... NO ERRORS - UPDATE MASCON ON PSS
    TEXT, TEMP, [GROUP = 227, GDIV].
    TEXT, TEMP, [OWNER = GRANT,K].
    TEXT, TEMP, [CHANGE LIBRARY = MASCON].
    TEXT, TEMP, [DESTROY SUBSET = MSCNPLO].
    TEXT, TEMP, [RENAME SUBSET MSCNPL=MSCNPLO].
(5) TEXT, TEMP, [CREATE SUBSET = MSCNPL].
    TEXT, TEMP, [COPY 0 F FROM FILE = MSCNPL].
    TEXT, TEMP, [REPLACE SUBSET = MSCNBN].
    TEXT, TEMP, [COPY 0 F FROM FILE = MSCNBN].
    TEXT, TEMP, [REPLACE SUBSET = MSCNSYM].
    TEXT, TEMP, [COPY 0 F FROM FILE = MSCNSYM].
    TEXT, TEMP, [END].
    COPY, TEMP/RX, OFXB, CPSSIN/RR.
     .
    COPYPSS, CPSSIN.
    RETURN, CPSSIN.
    ENTERPS, MASCON, MSCNPL, MSCNPL.
    ENTERPS, MASCON, MSCNBN, MSCNBN.
    ENTERPS, MASCON, MSCNSYM, MSCNSYM.
     .
     .
     .
    ..... CREATE AN ARCHIVE FILE OF THIS MASCON UPDATE FOR OUTPUT
    ..... AS MICROFICHE.
    EXIT.
    CXIT.
    FIN.
    ENDSKIP.
    SFL, 50000, 0.
    TIM.
    DDB.
    FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
    REWIND, DAYFILE.
    FISHTLT, DAYFILE.
    TEXT, ARCHIVE, [$RU].
    TEXT, ARCHIVE, [$B=DAYFILE].
    COPY, DAYFILE/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=INPUT].
    REWIND, INPUT.
    COPYSBF, INPUT, ARCHIVE.
    RETURN, INPUT.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=OUTPUT].
    COPY, OUTPUT/RR, ARCHIVE.
    COPY, LIST/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=SYMLIST].
    COPY, SYM/RX, ARCHIVE.
    DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
    +T2=[→R6→R7→R8→R9].
```

FIGURE J-14. Continued.

1. Job Card — The job card should contain your name and LBL account number.

2. Routing Information — The routing instructions should contain your address.

3. Title Card — The title should be whatever you want.

4. Data Retrieval — The LIBCOPY card that retrieves CMOD should retrieve your valid FTN UPDATE deck.

5. Data Storage — The archiving instructions should send the recompiled files to the appropriate archive.

Figure J-15 lists a sample LR1SCD, the control card deck that recompiles LIRAQ-1S. The following cardsshould be modified before executing LR1SCD.

1. Job Card — The job card should contain your name and LBL account number.

2. Routing Information — The routine instructions should give your address.

3. Title Card — The title should be whatever you wish.

4. Data Retrieval — The LIBCOPY card that fetches L1MOD, the UPDATE deck, should fetch your valid FTN UPDATE deck.

Figure J-16 lists a sample LR2SCD, the control card deck that recompiles LIRAQ-2S. The five indicated changes should be modified before running this deck:

1. Job Card — The job card should have your name and job number.

2. Routing Information — The routine instructions should have your address.

3. Title Card — The title should be altered to your choice.

4. Data Retrieval — Your valid L2MOD UPDATE deck should be recovered from archive.

5. Data Storage — The recompilation should be stored in your archive.

Figure J-17 gives a sample of VERFUCA, the deck that recompiles VERF. VERFUCA must be modified as follows:

1. Job Card — Have the user's name and account on the job card.

2. Routing Information — Have the user's address in the routing instructions.

3. Title Card — The title should be altered to your choice.

4. Data Storage — Store the new compilation in the user's archive.

5. After card 55 append the described update decks, identifier, and accounted special control cards.

```
(1) LR1S,7,500.679656,GRANT,K
    *HOLDOUT
    *PSS
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .≠ LIRAQ1S UPDATE AND COMPILATION
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE UPDATE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .  AVAILABILITY...
    .        THIS CONTROL DECK MAY BE OBTAINED BY EXECUTING THE CONTROL
    .        CARD
    .           FETCHPS, LIRAQ, LR1SCD, LR1SCD.
    .
    .  PURPOSE...
    .        THIS DECK PERFORMS THE FOLLOWING TASKS -
    .           1) UPDATES THE LIRAQ1 PROGRAM LIBRARY 'LR1SPL' FROM
    .              DIRECTIVES ON THE FILE 'L1MOD'.
    .           2) GENERATES A RELOCATABLE BINARY FILE 'LR1SBN'
    .           3) GENERATES A GRUMP SYMBOL TABLE FILE 'LR1SSYM'
    .
    .        THE FILE 'L1MOD' CONTAINS THE MODIFICATIONS TO BE MADE TO
    .        'LR1SPL'.  AS EACH 'L1MOD' DECK IS RUN, IT SHOULD BE ARCHIVED
    .        TO A PSS SUBSET WHOSE NAME IS OF THE FORM 'L1YMMDD', WHERE
    .        DD=DAY, MM=MONTH, AND Y=LAST DIGIT OF THE YEAR.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .
    DISKHOG, 20000.
    FETCHPS, LIRAQ, OLDPL, LR1SPL.
    .**** THE FOLLOWING CARD IS UPDATE DEPENDENT.  MAKE SURE THAT IT
    .**** FETCHES THE LATEST UPDATE WHICH IS TO BE APPLIED TO THE LIRAQ1S
    .**** PROGRAM LIBRARY.
(4) LIBCOPY, LIRAQ, L1MOD, L1MOD.
    .
    .
    ..... GENERATE THE COMPILE FILE AND CREATE A NEW PROGRAM LIBRARY
    TEXT, LIST, [$B=UPDATE].
    UPDATE, F, I=L1MOD, LC=10000, N=LR1SPL, O=LIST.
    RETURN, L1MOD, OLDPL.
    FTN4, B=LR1SBN, I=COMPILE, L=COMP, LCM=I, OPT=2, R=3.
    CXIT.
    COPY, COMP/RR, LIST.
    BGNSKIP.
    FIN.
    RETURN, COMPILE.
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=COMPILE].
    COPY, COMP/RR, LIST.
    .
    .
    ..... TEST LOAD THE NEW BINARY FILE
    GETTAPE, ULIB=IDDSTST/ULIB, 16964, DATE=02DEC78.
    GETTAPE, SCLGOF=GRAPHIC/SCLGOF, 16964, DATE=02DEC78.
    GETTAPE, TV80TLB=GRAPHICS/TV80TLB, 16964, DATE=02DEC78.
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=LOADMAP].
    LINK, F=LR1SBN, F=SCLGOF, L=LIST, LO=BERX, P=ULIB, P=TV80TLB.
```

FIGURE J-15. Sample of LR1SCD, the control card deck that recompiles LIRAQ-1S.

```
    RETURN, SCLGOF, TV80TLB, ULIB.
    SFL, 50000,0.
    .
    .
    ..... GENERATE THE SYMBOL TABLE
    GRUMP, L=0, P=COMP, WSYM=LR1SSYM.
    RETURN, COMP.
    REWIND, LR1SBN.
    SYMLIST, LR1SBN, SYM.
    .
    .
    ..... NO ERRORS - UPDATE LIRAQ1S ON PSS
    TEXT, TEMP, [GROUP = 227, GDIV].
    TEXT, TEMP, [OWNER = JOHNSTON,W].
    TEXT, TEMP, [CHANGE LIBRARY = LIRAQ].
    TEXT, TEMP, [DESTROY SUBSET = LR1SPLO].
    TEXT, TEMP, [RENAME SUBSET LR1SPL=LR1SPLO].
    TEXT, TEMP, [CREATE SUBSET = LR1SPL].
(5) TEXT, TEMP, [COPY 0 F FROM FILE = LR1SPL].
    TEXT, TEMP, [REPLACE SUBSET = LR1SBN].
    TEXT, TEMP, [COPY 0 F FROM FILE = LR1SBN].
    TEXT, TEMP, [REPLACE SUBSET = LR1SSYM].
    TEXT, TEMP, [COPY 0 F FROM FILE = LR1SSYM].
    TEXT, TEMP, [END].
    COPY, TEMP/RX, OFXB, CPSSIN/RR.
    .
    COPYPSS, CPSSIN.
    RETURN, CPSSIN.
    ENTERPS, LIRAQ, LR1SPL, LR1SPL.
    ENTERPS, LIRAQ, LR1SBN, LR1SBN.
    ENTERPS, LIRAQ, LR1SSYM, LR1SSYM.
    .
    .
    ..... CREATE AN ARCHIVE FILE OF THIS LIRAQ1S UPDATE FOR OUTPUT
    ..... AS MICROFICHE.
    EXIT.
    CXIT.
    FIN.
    ENDSKIP.
    SFL, 50000, 0.
    TIM.
    DDB.
    FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
    REWIND, DAYFILE.
    FISHTLT, DAYFILE.
    TEXT, ARCHIVE, [$RU].
    TEXT, ARCHIVE, [$B=DAYFILE].
    COPY, DAYFILE/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=INPUT].
    REWIND, INPUT.
    COPYSBF, INPUT, ARCHIVE.
    RETURN, INPUT.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=OUTPUT].
    COPY, OUTPUT/RR, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    COPY, LIST/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=SYMLIST].
    COPY, SYM/RX, ARCHIVE.
    DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],

    +T2=[→R6→R7→R8→R9].
```

FIGURE J-15. Continued

```
(1) LR2S,7,500.679656,GRANT,K
    *HOLDOUT
    *PSS
    *NOTAPES
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .# LIRAQ2S UPDATE AND COMPILATION
    .**** THE PRECEEDING TWO CARDS ARE RUN DEPENDENT.  THE FIRST CARD
    .**** CONTAINS INFORMATION FOR ROUTING OF JOB OUTPUT.  THE SECOND
    .**** CARD CONTAINS THE UPDATE TITLE FOR LABELING OF JOB OUTPUT.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .     THIS DECK PERFORMS THE FOLLOWING TASKS -
    .     1) UPDATES 'LR2SPL' FROM MODS ON 'L2MOD'
    .     2) GENERATES THE BINARY AND 'GRUMP' SYMBOL TABLE FOR LIRAQ2S
    .
    .     CONVENTIONS -
    .     1) THIS DECK IS TO BE RUN ONCE FOR EACH SET OF TESTED MODS
    .        ('L2MOD' DECK).
    .     2) THE FILE 'L2MOD' CONTAINS THE MODS TO BE MADE TO 'LR2SPL'.
    .     3) AS EACH 'L2MOD' DECK IS RUN, IT SHOULD BE ARCHIVED TO A
    .        PSS SUBSET WHOSE NAME IS OF THE FORM 'L2YMMDD', WHERE
    .        DD=DAY, MM=MONTH, Y=LAST DIGIT OF THE YEAR.
    .
    .XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
    .
    .
    DISKHOG, 20000.
    FETCHPS, LIRAQ, OLDPL, LR2SPL.
    .**** THE FOLLOWING CARD IS UPDATE DEPENDENT.  MAKE SURE THAT IT
    .**** FETCHES THE LATEST UPDATE WHICH IS TO BE APPLIED TO THE LIRAQ2S
    .**** PROGRAM LIBRARY.
(4) LIBCOPY, LIRAQ, L2MOD, L2MOD.
    .
    .
    ..... GENERATE THE COMPILE FILE AND CREATE A NEW PROGRAM LIBRARY
    TEXT, LIST, [$B=UPDATE].
    UPDATE, F, I=L2MOD, LC=10000, N=LR2SPL, O=LIST.
    RETURN, L2MOD, OLDPL.
    FTN4, B=LR2SBN, I=COMPILE, L=COMP, LCM=I, OPT=2, R=3.
    RETURN, COMPILE.
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=COMPILE].
    COPY, COMP/RR, LIST.
    .
    .
    ..... TEST LOAD THE NEW BINARY FILE
    GETTAPE, ULIB=IDDSTST/ULIB, 16964, DATE=02DEC78.
    GETTAPE, SCLGOF=GRAPHIC/SCLGOF, 16964, DATE=02DEC78.
    GETTAPE, TV80TLB=GRAPHICS/TV80TLB, 16964, DATE=02DEC78.
    TEXT, LIST, [$CL].
    TEXT, LIST, [$B=LOADMAP].
    LINK, F=LR2SBN, F=SCLGOF, L=LIST, LO=BERX, P=ULIB, P=TV80TLB.
    RETURN, SCLGOF, TV80TLB, ULIB.
    SFL, 50000,0.
    .
    .
    ..... GENERATE THE SYMBOL TABLE
    GRUMP, L=0, P=COMP, WSYM=LR2SSYM.
    RETURN, COMP.
    REWIND, LR2SBN.
```

FIGURE J-16. Example of LR2SCD, the control card deck that recompiles LIRAQ-2S.

```
    SYMLIST, LR2SBN, SYM.
    .
    .
    ..... NO ERRORS - UPDATE LIRAQ2S ON PSS
    TEXT, TEMP, [GROUP = 227, GDIV].
    TEXT, TEMP, [OWNER = JOHNSTON,W].
    TEXT, TEMP, [CHANGE LIBRARY = LIRAQ].
    TEXT, TEMP, [DESTROY SUBSET = LR2SPLO].
    TEXT, TEMP, [RENAME SUBSET LR2SPL=LR2SPLO].
    TEXT, TEMP, [CREATE SUBSET = LR2SPL].
(5) TEXT, TEMP, [COPY 0 F FROM FILE = LR2SPL].
    TEXT, TEMP, [REPLACE SUBSET = LR2SBN].
    TEXT, TEMP, [COPY 0 F FROM FILE = LR2SBN].
    TEXT, TEMP, [REPLACE SUBSET = LR2SSYM].
    TEXT, TEMP, [COPY 0 F FROM FILE = LR2SSYM].
    TEXT, TEMP, [END].
    COPY, TEMP/RX, OFXB, CPSSIN/RR.
    .
    COPYPSS, CPSSIN.
    RETURN, CPSSIN.
    ENTERPS, LIRAQ, LR2SPL, LR2SPL.
    ENTERPS, LIRAQ, LR2SBN, LR2SBN.
    ENTERPS, LIRAQ, LR2SSYM, LR2SSYM.
    .
    .
    ..... CREATE AN ARCHIVE FILE OF THIS LIRAQ2S UPDATE FOR OUTPUT
    ..... AS MICROFICHE.
    EXIT.
    CXIT.
    FIN.
    SFL, 50000, 0.
    TIM.
    DDB.
    FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
    REWIND, DAYFILE.
    FISHTLT, DAYFILE.
    TEXT, ARCHIVE, [$RU].
    TEXT, ARCHIVE, [$B=DAYFILE].
    COPY, DAYFILE/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=INPUT].
    REWIND, INPUT.
    COPYSBF, INPUT, ARCHIVE.
    RETURN, INPUT.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=OUTPUT].
    COPY, OUTPUT/RR, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    COPY, LIST/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=SYMLIST].
    COPY, SYM/RX, ARCHIVE.
    DISPOSE, ARCHIVE=MF, T1=[→R0→R1→R2→R3→R4→R5],
    +T2=[→R6→R7→R8→R9].
```

FIGURE J-16. Continued.

```
(1) VERF,16,120.692356,GRANT,K
    *HOLDOUT
    *PSS
(2) (EXPEDITOR SERVICES/WILLIAM H. DUEWER/L-262/LLL
(3) .≠ VERF UPDATE, COMPILE, AND LOAD
    TEXT, OUTPUT, [$CL].
    TEXT, OUTPUT, [$B=UPDATE].
    FETCHPS, LIRVERF, OLDPL, VERFPL.
    UPDATE, F, I=INPUT, N=VERFPL.
    RETURN, OLDPL.
    TEXT, OUTPUT, [$CL].
    TEXT, OUTPUT, [$B=COMPILE].
    FTN4, I=COMPILE, OPT=2, R=3.
    RETURN, COMPILE.
    TEXT, OUTPUT, [$CL].
    TEXT, OUTPUT, [$B=LOAD].
    GETTAPE, SCLGOF=GRAPHIC/SCLGOF, 16964, DATE=02DEC78.
    GETTAPE, ULIB=IDDSTST/ULIB, 16964, DATE=02DEC78.
    LINK, F, F=SCLGOF, LO=BERX, P=ULIB.
    RETURN, SCLGOF, ULIB.
    .
    . SAVE NEW PROGRAM LIBRARY AND RELOCATABLE BINARY
   [LIBRITE, LIRVERF, VERFPL, VERFPL, 227, W=[GRANT,K].
(4)|LIBRITE, LIRVERF, LGO, VERFBN, 227, W=[GRANT,K].
   |ENTERPS, LIRVERF, VERFPL, VERFPL.
   LENTERPS, LIRVERF, LGO, VERFBN.
    RETURN, VERFPL, VERFBN.
    CXIT.
    END.
    EXIT.
    END.
    FIN.
    TEXT, ARCHIVE, [$RU].
    TEXT, ARCHIVE, [$B=DAYFILE].
    TIM.
    DDB.
    REWIND, DAYFILE.
    FETCHPS, GRAPHICS, FISHTLT, FISHTLT.
    FISHTLT, DAYFILE.
    RETURN, FISHTLT.
    COPY, DAYFILE/RX, ARCHIVE.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=VERFUCA].
    REWIND, INPUT.
    COPYSBF, INPUT, ARCHIVE.
    RETURN, INPUT.
    TEXT, ARCHIVE, [$CL].
    TEXT, ARCHIVE, [$B=OUTPUT].
    COPY, OUTPUT/RB, ARCHIVE.
    DELETE, OUTPUT.
    DISPOSE, ARCHIVE=MF,
    + T1 = [  UCRL-52864, DUEWER ET AL, LIRAQ APPLICATION TO ST. LOUIS ],
    + T2 = [  (VERF COMPILATION)                           11/79 48X 12 OF 29 ].
    END.
    */ UPDATE DECKS, IDENTS, AND CONTROL CARDS
   [*IDENT 791119
   |*INSERT ICON.249
(5)|       NSTOB=0
   |       NWXMX=0
   |       NWYMX=0
   L
```

FIGURE J-17. Example of VERFUCA, the control card deck that recompiles VERF.

APPENDIX K

APPROXIMATE COST OF RUNNING THE LIRAQ MODELS AND THEIR ASSOCIATED DATA PROCESSING ROUTINES

A significant portion of the cost of running the LIRAQ codes at LBL is in the graphics routines. As a result, the costs of running LIRAQ-2 and MASCON can be reduced by reducing the amount of graphical output requested. Also, the time demands of LIRAQ-1, LIRAQ-2, and MASCON vary substantially as a function of model grid interval, meteorological update interval, and, for LIRAQ-2, the details of the intitial concentration fields for O_3 and NO. Table K-1 lists the various codes, the CPU costs as of December 1978, and the dollar costs we have experienced.

This section will list approximate total computing unit costs for typical executions of the various processors, and recommend a minimum computing unit allowance for execution of the codes. Because only LIRAQ-2S retains information needed to continue a problem if it is aborted, it is desirable to allow a fairly generous margin of error in estimating run times. It is expensive and frustrating to spend several thousand computing units only to have a problem abort in the final stages of execution because of an underestimated time limit. In general, it would be wise to exceed the estimated actual costs by a factor of about 2, however very large jobs are run more slowly than are ordinary jobs. Thus, it is advisable to reduce the margin of error once you have experience in running a given code.

The only codes to be run as part of LIRAQ that should ever have running costs in excess of 1000 CPU are the source processor, MASCON, LIRAQ-1S and LIRAQ-2S. Under normal operating procedures plausible for an air quality management district, the source processor would be run rarely if at all. In any case, the only way to minimize the source processor costs is to avoid grids with large numbers of grid elements.

MASCON costs are minimized by avoiding graphics. If the user wishes to use one day for an extensive study, he should certainly use the full graphical output from MASCON. Under such circumstances LIRAQ will probably be run more frequently than MASCON so that MASCON costs will be a small portion of total costs. However, if the user is running several days in a pure verification mode it may be desirable to reduce costs by suppressing the MASCON graphics. This should reduce costs by $\sim$400-1000 CPU (depending on grid, edit interval, etc.). By supressing graphics MASCON costs should be reduced 40-80%.

LIRAQ-1S costs vary directly with he number of grid elements, number of species, and number of hours to be simulated. When the highest flux velocity in the grid exceeds $(\Delta x\ (m))/(600\ (sec))$ the cost will be almost inversely proportional to Δx and almost directly proportional to maximum flux velocity. Thus, to minimize LIRAQ-1 costs, avoid using larger than necessary grids, avoid using more resolution

TABLE K-1. Processors associated with LIRAQ and their running costs.

Code	Function	CU costs* Total	$ costs** 1978	Allow
UADATA	Graphical display of RAMS data (also compiles code)	450-600	$30-40	800
Q-Processor	Generation of QICON RAMS processing	30-40	$3	100
Q-Processor-Compilation	Compilation of Q-Processor (not routinely done)	40	$3-4	60
M-Processor	Averages RAMS data	20-40	$2-4	60
M-Processor-Compilation	(Not routinely done)	40	$3-4	60
MASCON	Generation of QTRAN files	80-1200	$6-100	400-2000
	Without graphics MASCON costs should rarely exceed 400 CUs. With graphics, even minimum graphics, costs will be in the 500-1500 CU range. Costs will be in the lower end of the cited range for smaller numbers of grid elements and nearly consistent input fields, costs will be higher for larger numbers of grid elements, more complex terrain, and less consistent input fields.			
MASCON-Compilation	Not routinely done	150	$10-20	200
Source Processor	Generate QSORfiles	500-1200	$30-100	800-2000
	Source processor costs are higher for small grid intervals, larger numbers of grid elements. Allow 800 CUs for 5 km grid, 2000 for 1 km grid.			
Source Processor-Compilation	Not routinely done	50-100	$5-10	100
LIRAQ-1S	Compute concentrations of chemically inactive species	300-6000*	$30-600	1000-10000
	LIRAQ-1S costs are nearly proportional to number of species times number of grid elements times number of time steps. Time steps are often controlled by a Courant condition for small grid intervals and/or high winds. Allow 3000 CPUs for a 5 km 25 x 25 grid, 2 pollutants, and 24 hours of normal meteorology. Increase CU allowance for more species, larger grid, or abnormally high winds.			

than is really useful, and avoid running unnecessary pollutants or simulating over intervals that are longer than necessary.

TABLE K-1. Continued.

Code	Function	CU costs* Total	$ costs** 1978	Allow
LIRAQ-1S-Compilation	Not routinely done	120	$7-10	300
LIRAQ-2S	Compute concentrations of chemically active pollutants	12,000-20,000	$500-1200	25,000
	Costs are dependent on start time, stop time, and (if start is before sunrise) initial O_3 and NO concentrations. Costs will be 12000-14000 CUs to run from just after sunrise to just before sunset. Costs will be 16000-22000 CUs to run from $\sim$1-2 hours before sunrise to just before sunset. Cost to run 24 hours is estimated to be $\sim$40,000 CUs. Costs can be reduced by avoiding start times before sunrise, stop times after sunset, and NO and ozone initial concentrations that are incompatible at night. Really incompatible O_3 and NO initial fields might cause the code to spend $\sim$ 25000 CUs to run one hour before sunrise. Costs can also be lowered by running over the weekend or at deferred priorities.			
LIRAQ-2S-Compilation	Not routinely done	200	$10-15	300
VERF	Compare model with observation	200-300	$10-15	500
VERF-Compilation	Not routinely done	100	$5-7	200

*LBL computing unit costs experienced in November and December, 1978.

**Approximate dollar costs assuming standard priority runs at LBL based on our experience in late 1978 and early 1979.

***Recommended computing unit allowance for a typical problem. We recommend that a new user test himself on LIRAQ-2S by running a one-hour problem starting after sunrise with a 3000 CU limit to avoid high costs if the input data are bad, or if LIRAQ-2S has been affected by changes in the LBL compiler or loader (as has happened on occasion in the past).

The costs of running LIRAQ-2S will normally exceed the costs of all other routines combined and by a substantial margin. Figure K-1 displays actual CPU time vs. model hour for two different simulations. It is evident that it is more expensive to run before sunrise than after, and that a considerable overhead occurs whenever new meteorological data are read. Also, the higher costs recorded for the first half hour of every hour for which new meteorological data are not input reflects the cost of generating the extensive LIRAQ graphical and tabular output. I/O appears to account for about 40-60% of LIRAQ-2S costs at LBL. LIRAQ costs can be minimized by starting the problem after sunrise and terminating before sunset, by updating the

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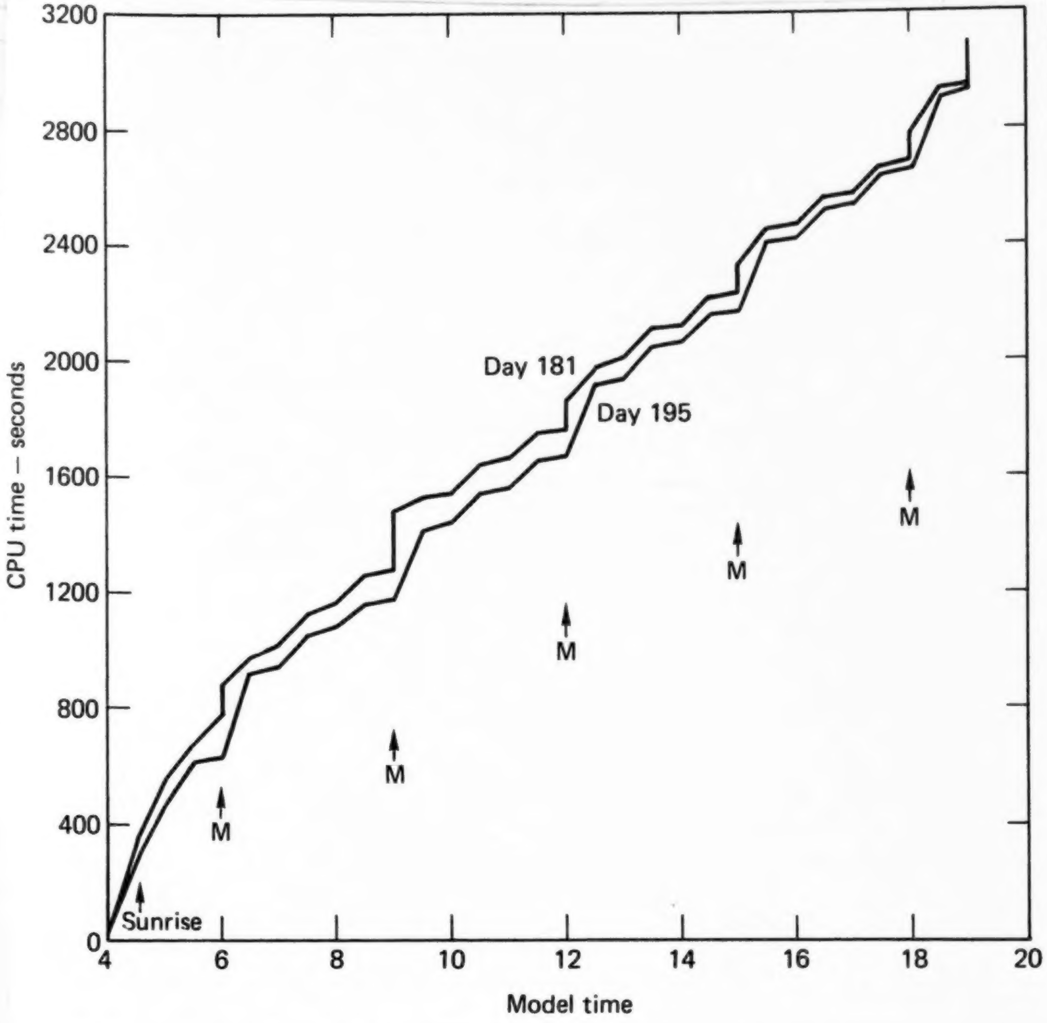

FIGURE K-1. CPU time vs. model time for two LIRAQ-2S runs. In the simulation of day 181 YOUT was called before and after QTRAN and QSOR were read and graphical output was produced at meteorological update times. The vertical portions of that plot at meteorological update times (marked with an "M") reflect the cost of I/O associated with meteorological updates. The heavy computer usage in the first half of any non-meteorological update hour reflects the extra cost of producing QGRAPH and QHSP output.

meteorology at 3 hour intervals, by not requiring graphical output for species that will not be examined (e.g., one might not need to output all three LIRAQ hydrocarbon classes, one might suffice). One might supress SO_2 and/or $SO_4^=$ if there is little verification data for those species, since LIRAQ is not well designed to treat materials dominated by elevated point sources.

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